

Accelerated Inorganic Electride Discovery by Generative Models and Hierarchical Screening

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Electrides are exotic compounds in which excess electrons occupy interstitial regions of the crystal lattice and serve as anions, exhibiting exceptional properties such as low work function, high electron mobility, and strong catalytic activity. Although they show promise for diverse applications, identifying new electrides remains challenging due to the difficulty of achieving energetically favorable electron localization in crystal cavities. Here, we present an accelerated materials discovery framework that combines physical principles, diffusion-based materials generation with hierarchical thermodynamic and electronic structure screening. Using this workflow, we systematically explored 1510 binary and 6654 ternary chemical compositions containing excess valence electrons from electropositive alkaline, alkaline-earth, and early transition metals, and then filtered them with a high-throughput validation on both thermodynamical stability and electronic structure analysis. As a result, we have identified 264 new electron-rich compounds within 0.05 eV/atom above the convex hull at the density functional theory level, including 13 thermodynamically stable electrides. Our approach demonstrates a generalizable strategy for targeted materials discovery in a vast chemical space.

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I. INTRODUCTION

Electrides represent a unique class of ionic crystals in which electrons occupy interstitial regions of the crystal lattice and serve as the nucleus-free anionic species [1,2]. Since the first crystalline electride $\text{Cs}^+(18\text{-crown-6})_2\text{e}^-$ was reported [3], these materials have received continuous attention owing to their unusual electronic properties and promising applications in various electronic devices and chemical reactions [4].

While early electride research focused primarily on organic compounds [5–7], these materials suffer from thermal instability above room temperature and sensitivity to moisture, severely limiting their practical applications [2]. In 2003, Hosono and co-workers achieved a significant progress toward the realization of inorganic electrides by the successful synthesis of $\text{Ca}_6\text{Al}_7\text{O}_{16}$ (C12A7:2e^-) via oxygen-reducing processes from the mineral mayenite ($12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$) [8]. The discovery of thermally stable C12A7:2e^- has stimulated extensive efforts to exploit these materials to enable new technology applications such as ammonia synthesis [9–11] and electron emission [12], as well as to search for other inorganic electrides [4,13,14].

Based on the dimensionality of anionic electron distribution, electrides can be classified into zero-dimensional (0D), one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D) categories, each exhibiting unique electronic and transport characteristics. Among these, the 2D electride Ca_2N has attracted considerable attention due to its high electron mobility, low work function, and striking anisotropic magnetoresistance [15,16]. The Ca_2N structure type ($R\bar{3}m$: 166) with an anti- CdCl_2 layered structure represents a particularly promising structural family for 2D electride formation, including Sr_2N , Ba_2N , and Y_2C [17–19]. Similarly, the 1D electrides of the Mn_5Si_3 -type have been widely studied due to their peculiar semiconducting and superconducting behaviors [20–23].

Beyond the chemical novelty, electrides have also emerged as a promising platform for realizing topological electronic phases. Recent theoretical work has demonstrated that the weakly bound anionic electrons near the Fermi level in electrides naturally facilitate band inversions necessary for topological insulating and semimetal phases. Several electrides including Y_2C , Sc_2C , Sr_2Bi , and HfBr have been predicted to exhibit nontrivial topological properties such as nodal-line semimetal states, quantum spin Hall effects, and even quantum anomalous Hall insulator behavior [24–26]. High-pressure studies have further expanded the electride landscape, revealing that simple metals like sodium and lithium can transform into insulating electride phases under extreme compression, where valence electrons migrate to interstitial sites and form quasiatomic or quasimolecular units [27–31].

To date, the number of experimentally confirmed electrides remains small compared to the vast chemical space of

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potential candidates. This scarcity has motivated further computational efforts for new electrider discovery through high-throughput screening of existing crystal structure databases [17,32–34]. Tada *et al.* pioneered high-throughput screening of approximately 34 000 materials from the Materials Project, employing three key indicators: positive total formal charge, layered structures for two-dimensionality, and empty interlayer spaces to search for new 2D electrideres [17]. Building on this foundation, Burton *et al.* performed automated density functional theory (DFT) calculations on over 60 000 compounds from the Materials Project to identify 65 new electrider candidates [32]. This number was further expanded to 167 by Zhu *et al.* through a more comprehensive pipeline that accounts for electron localization analysis in both spatial and energy space [34,35]. Additionally, structure engineering based on existing materials has been applied to discover new electrideres using simple structural prototypes [36,37] or complex zeolite frameworks [38,39].

While database screening has proven invaluable for identifying electrideres from existing material prototypes, it is also appealing to design and discover new electrideres in unexplored chemical space. Hence, crystal structure prediction methods based on global optimization algorithms have been attempted in various ways [18–20,40]. Zhang *et al.* developed an inverse-design method to identify 24 stable and 65 metastable new inorganic electrideres covering 33 distinct prototypes [19]. Wang *et al.* combined *ab initio* structure searches with experimental validation to synthesize Sr_5P_3 , a 1D semiconducting electrider [20]. Zhu *et al.* computationally designed flexible electrideres Rb_3O and K_3O with nontrivial band topology, demonstrating that multiple types of cavities enable tuning of anionic electron spatial arrangements [40]. These results collectively demonstrate that it is possible to identify truly new electrideres that may not been synthesized in the past. However, they were mostly limited to a few chemical systems and compositions due to the concerns of computational cost.

Despite these exciting developments in theory-driven discovery [20,37,41], identifying new electrideres remains a grand challenge due to three main obstacles. First, determining which chemical space to explore is critical since it is infeasible to systematically sample all possible combinations across the whole periodic table of over 100 elements. Once the chemical space is determined, it is essential to develop a sustainable framework capable of rapidly performing two critical tasks: (1) predicting all energetically favorable crystal structures within a given chemical space and (2) evaluating their thermodynamic feasibility and relevant properties. To date, most existing methods applied to electrider research heavily rely on DFT-based electronic structure calculations for both tasks, but they are not suitable for systematic exploration study due to their prohibitive computational costs.

Fortunately, recent advances in machine learning (ML) and artificial intelligence (AI) have revolutionized materials discovery and evaluation [42,43]. Diffusion-based generative models [43–46] enable efficient exploration of crystal structure space by learning data-driven representations, generating diverse low-energy structures orders of magnitude faster than traditional global optimization methods. Concurrently, ML foundation model interatomic potentials [47–49]

have dramatically accelerated structural evaluation, providing near-DFT accuracy at computational costs reduced by 3–4 orders of magnitude. This convergence of advances in generative AI and ML potentials enables targeted exploration of well-defined chemical spaces that would be computationally prohibitive using conventional approaches. While some concerns have been raised regarding the novelty of AI-based crystal generation [50], these methods have been applied to catalyze discoveries across diverse functional materials including magnets [43] and thermoelectrics [51–53].

In this work, we demonstrate a computational framework for efficient exploration of large chemical space, using inorganic electrider discovery as a case study. Crucially, we began with chemical space selection based on physical principles of electrider formation, focusing on binary and ternary compositions with excess valence electrons from electropositive metals. We then employed MatterGen generative model [43] and foundation interatomic potentials MatterSim [47] to rapidly screen structures in the reduced chemical space. This was further integrated with our previously developed high-throughput electronic structure framework [40] to identify low-energy electrideres. Our results demonstrate the power of generative AI and ML to accelerate targeted materials discovery and provide a generalizable strategy for future explorations beyond electrideres.

The remainder of this paper is organized as follows. Section II describes our computational methodology in detail, including targeted chemical space selection, generative structure prediction, and the hierarchical screening workflow combining ML prescreening with DFT validation for electrider identification. Section III presents our discoveries of binary and ternary electrider candidates, analyzing their structural characteristics, thermodynamic stability, and electronic structure features, with emphasis on interstitial electron localization patterns and prototype recurrence across chemical space. Section IV discusses the implications of our findings for rational electrider design principles, followed by concluding remarks and perspectives on how generative models and machine learning potentials enable targeted exploration of vast chemical space for accelerated materials discovery.

II. COMPUTATIONAL METHODS

Figure 1 outlines our electrider discovery workflow, including (1) generating candidate structures across targeted electron-rich compositions using the MatterGen model, (2) relaxing the generated structures and performing thermodynamical stability analysis to select low-energy candidates ($E_{\text{ref-hull-MLP}}$) via machine learning potentials, (3) performing high-throughput structural optimization and electronic structure analysis using DFT to identify the potential electrideres, and (4) conducting high-precision DFT calculations for promising electrider candidates to obtain accurate final energetics ($E_{\text{hull-DFT}}$). Below, we describe each stage in detail.

A. Stage 1: Chemical space exploration

In the past, crystalline interstitial electrons are commonly found in environments dominated by electropositive metals [19,34,35,54], including alkaline, alkaline-earth, and early

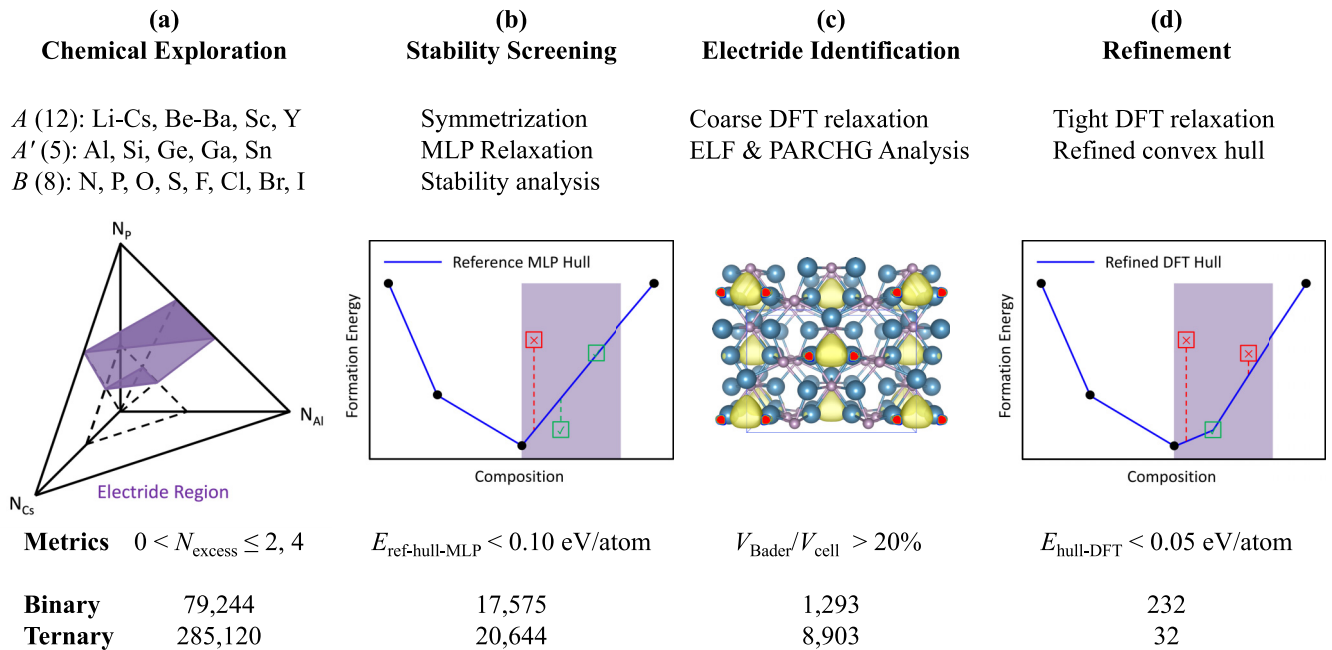


FIG. 1. The workflow for accelerated electrider discovery combining physical principles, generative modeling (MatterGen), machine learning potential prescreening (MatterSim), and high-throughput DFT validation for electrider and stability analysis. The top panel outlines key operations at each stage, the middle panel illustrates the definition of metrics used for candidate selection with the targeted compositions being highlighted by the light purple color, and the bottom panel specifies filtering criteria and the number of candidates retained after each stage.

transition metals. This observation strongly suggests that these electropositive metals are essential for providing excess electrons and achieving the interstitial anionic electrons in the surrounding low-affinity nucleus. Consequently, we focused our exploration on binary (AB) and ternary ($AA'B$) compounds with excess valence electrons from 12 A -type electropositive metals (Li, Na, K, Rb, Cs, Be, Mg, Ca, Sr, Ba, Sc, Y) combined with 8 B -type electronegative nonmetals (N, P, O, S, F, Cl, Br, I). For ternary compositions, we additionally incorporated 5 A' -type Earth-abundant elements (Al, Si, Ge, Ga, Sn) to enhance structural and chemical diversity, encompassing a total of 96 binary and 480 ternary chemical systems. Exhaustive enumeration of all possible combinations with up to 20 atoms per unit cell would require sampling 190 discrete A_mB_n ($m+n \leq 20$) combinations per binary system and 1140 $A_mA'_lB_n$ ($l+m+n \leq 20$) combinations per ternary system, resulting in an astronomically large search space.

However, one does not have to explore all possible compositions. A common characteristic of electrideres is that the number of excess electrons should not only be positive but also remain moderate to avoid purely metallic behavior. Consequently, we restrict our search to compositions with no more than four excess electrons per formula unit for binaries and two for ternaries. Using empirical valence states (e.g., +2 for Ca and -2 for O), the number of excess electrons per formula unit is calculated as $N_{\text{excess}}(A_mB_n) = mV_A + nV_B$ and $N_{\text{excess}}(A_mA'_lB_n) = mV_A + lV_{A'} + nV_B$, where V_A , $V_{A'}$, and V_B are the valence states of elements A , A' , and B , respectively. Here, all compositions are enumerated as reduced (irreducible) formulas, and N_{excess} is evaluated per reduced formula unit. Thus, a composition such as A_8B_2 reduces to A_4B and is counted only once; its nonreduced multiples

enter only later, as supercells, during the generative step. The choice of a tighter window for ternaries ($0 < N_{\text{excess}} \leq 2$) reflects the much larger ternary search space (1140 versus 190 stoichiometric combinations per system). This restriction dramatically reduces the combinatorial search space. For example, Fig. 1(a) schematically shows that applying the constraint $0 < N_{\text{excess}} \leq 2$ to a ternary system (Cs-Al-P) can reduce the number of required stoichiometric combinations from 1140 to 50. Using this criterion, we kept 1510 binary and 6654 ternary compositions for further exploration.

Next, we retrained MatterGen [43], the state-of-the-art diffusion-based generative model using the Materials Project mp_20 dataset to generate new crystal candidates. The model was trained from scratch in the crystal structure prediction configuration, in which the only conditioning information is the target chemical composition. Importantly, no electrider-specific or any other property labels (e.g., work function, band gap, or interstitial-electron descriptors) were used during either training or sampling; the targeting of electrideres is achieved solely through the physically motivated composition selection above and the downstream screening below, not by biasing the generative model. For each target composition, we generated structures using multiple formula unit up to the ceiling of 20 atoms per unit cell. Specifically, each reduced formula was expanded to all valid supercell multiples within the 20-atom limit (e.g., a 6-atom A_4B_2 cell was generated at 6, 12, and 18 atoms/cell; a 9-atom A_6B_3 cell at 9 and 18 atoms/cell; and a 19-atom $A_{10}B_9$ cell at 19 atoms/cell only). The number of structures per composition is scaled with system size according to $N_{\text{attempts}} = 2 \times N_{\text{atoms per cell}}$ summed over its supercells. This setting eventually leads to a total of 79 244 binary and 285 120 ternary structures for MatterGen

generation. Using the NVIDIA A100 GPU, it approximately takes 1000 GPU hours, which is roughly consistent with the speed of 500 structures per GPU hour as reported in the original paper [43].

B. Stage 2: Stability screening

It is important to note that MatterGen only generates structures in the primitive cell setting without crystallographic symmetry information. To reduce the load for the follow-up relaxation, we symmetrized all generated structures using PyXtal [55] with a tolerance of 0.05 Å and then performed structural relaxations with the MatterSim machine learning potential (MLP) trained on Materials Project data [47]. Structures were relaxed in batches of 32 (configurable based on GPU memory availability) with calculator instance reuse to maximize GPU efficiency and minimize memory overhead. The relaxed structures were evaluated against reference convex hulls ($E_{\text{ref-hull-MLP}}$) using Materials Project data via pymatgen's Materials Application Programming Interface [56]. As illustrated in Fig. 1(b), a thermodynamically stable compound exhibits $E_{\text{ref-hull-MLP}} \leq 0$ eV/atom, while structures with $E_{\text{ref-hull-MLP}} \geq 0.10$ eV/atom can be discarded due to the unfavorable energy upon the decomposition to the reference stable compounds.

Next, a similarity check using pymatgen's structure matching algorithm was applied to remove duplicate structures with a site distance of 0.2, a fractional length tolerance of 0.2, and a lattice angle tolerance of 5°. This stage required approximately 400 GPU hours and yielded 17 575 unique binary and 20 644 ternary structures with $E_{\text{ref-hull-MLP}} < 0.10$ eV/atom for the next validation stage.

C. Stage 3: Electride characterization

Structures with $E_{\text{ref-hull-MLP}} < 0.10$ eV/atom were selected for further relaxation using VASP 6.2.1 [57], employing the Generalized Gradient Approximation functional according to Perdew *et al.* [58] with Projector augmented-wave pseudopotentials [59]. This DFT relaxation serves two purposes: first, to verify structural stability and ionic convergence in case the MLP relaxation was insufficient, and second, to re-evaluate the energy above hull using the relaxed structures. To reduce computational costs, we intentionally employed coarse settings for this stage (PREC = accurate, EDIFF = 10^{-6} eV, EDIFFG = -0.01 eV/Å for convergences, and NSW = 30, ISIF = 3, and POTIM = 0.3 for ion relaxation). This coarse DFT relaxation provides an efficient means to further filter out unstable structures exhibiting either nonphysical geometry or unfavorable energy ranking due to artifacts from the MLP prescreening.

Only successfully relaxed structures were retained for subsequent analysis, following our previously reported methodology for electride identification [34]. Specifically, we first computed the electron localization function (ELF) to identify whether electrons localize in interstitial sites. Upon identification of interstitial ELF maxima, we proceeded to compute five partial charge density (PARCHG) distributions, grouped into two complementary families: three energy-window files that integrate occupied states within $[E_F - \Delta E, E_F]$ for $\Delta E =$

0.025 eV ($e_{0.025}$), 0.5 eV ($e_{0.5}$), and 1.0 eV ($e_{1.0}$), which probe how the interstitial density builds up over progressively deeper energy ranges below the Fermi level; and two band-decomposed files for the top two valence bands (band₀ for the VBM and band₁ for VBM − 1), which isolate the band-resolved character of the interstitial electrons. For each PARCHG, the Bader algorithm partitioned electrons into basins based on zero-flux surfaces in the electron density gradient using the modified Bader utility [60], and the volume of any non-nuclear (interstitial) basin was recorded for each of the five files. A structure was first identified as an electride candidate when an interstitial basin was detected (nonzero volume) in at least one of the two near-Fermi energy windows and in either the deepest energy window or the top valence band, i.e., ($e_{0.025} > 0$ or $e_{0.5} > 0$) and ($e_{1.0} > 0$ or band₀ > 0). Requiring consistency between the energy-resolved and band-resolved descriptions ensures that the interstitial electrons are genuinely populated near the Fermi level rather than being an artifact of a single integration window.

As illustrated in Fig. 1(c), we subsequently retained the high-quality electrifieds by requiring a substantial interstitial volume fraction. For each PARCHG file, this fraction is defined as $f = 100 \times V_{\text{interstitial}}/V_{\text{cell}}$ (%), where $V_{\text{interstitial}}$ is the summed volume of the interstitial (non-nuclear) Bader basins and V_{cell} is the unit cell volume. Specifically, we required $\max(e_{0.025}, e_{0.5}, e_{1.0}) \geq 20\%$ and $\max(\text{band}_0, \text{band}_1) \geq 20\%$. This threshold is adopted from the volume-based topological analysis of Zhu *et al.* [34] and ensures that the interstitial electrons occupy a significant fraction of the unit cell, comparable to the volume fraction of a conventional anionic site, rather than being a negligible charge-transfer artifact. We verified that confirmed electrifieds comfortably exceed this threshold in the identical pipeline.

Using the initial detection criterion above, we identified a total of 1293 binary and 8903 ternary electride candidates, requiring approximately 20 000 CPU hours.

D. Stage 4: Refined DFT calculation

For promising electride candidates identified from stage 3, we further perform structural relaxation until it reaches the full convergence. These relaxed structures were recomputed using the PBE functional according to Materials Project's setting to obtain more accurate energy values, which ensures the correctness of the $E_{\text{ref-hull-DFT}}$ as compared to the reference values in the Materials Project. At this stage, we also updated the reference convex hull with the new results, as illustrated in Fig. 1(d). This eventually leads to the identification of 232 binary and 32 ternary electride compounds with the $E_{\text{hull-DFT}}$ values less than 0.05 eV/atom. This stage costs approximately 38 000 CPU hours. And all computed structural and property data are managed via the ASE's database utility [61]. We also computed phonons for a list of selected structures using the finite displacement method as implemented in the Phonopy code [62] to confirm the dynamical stability.

In general, this hierarchical screening framework strategically integrates physical principles with AI/ML tools for computational efficiency. First, we restrict our search to electron-rich compositions containing electropositive metals, thus greatly reducing combinatorial complexity. Second,

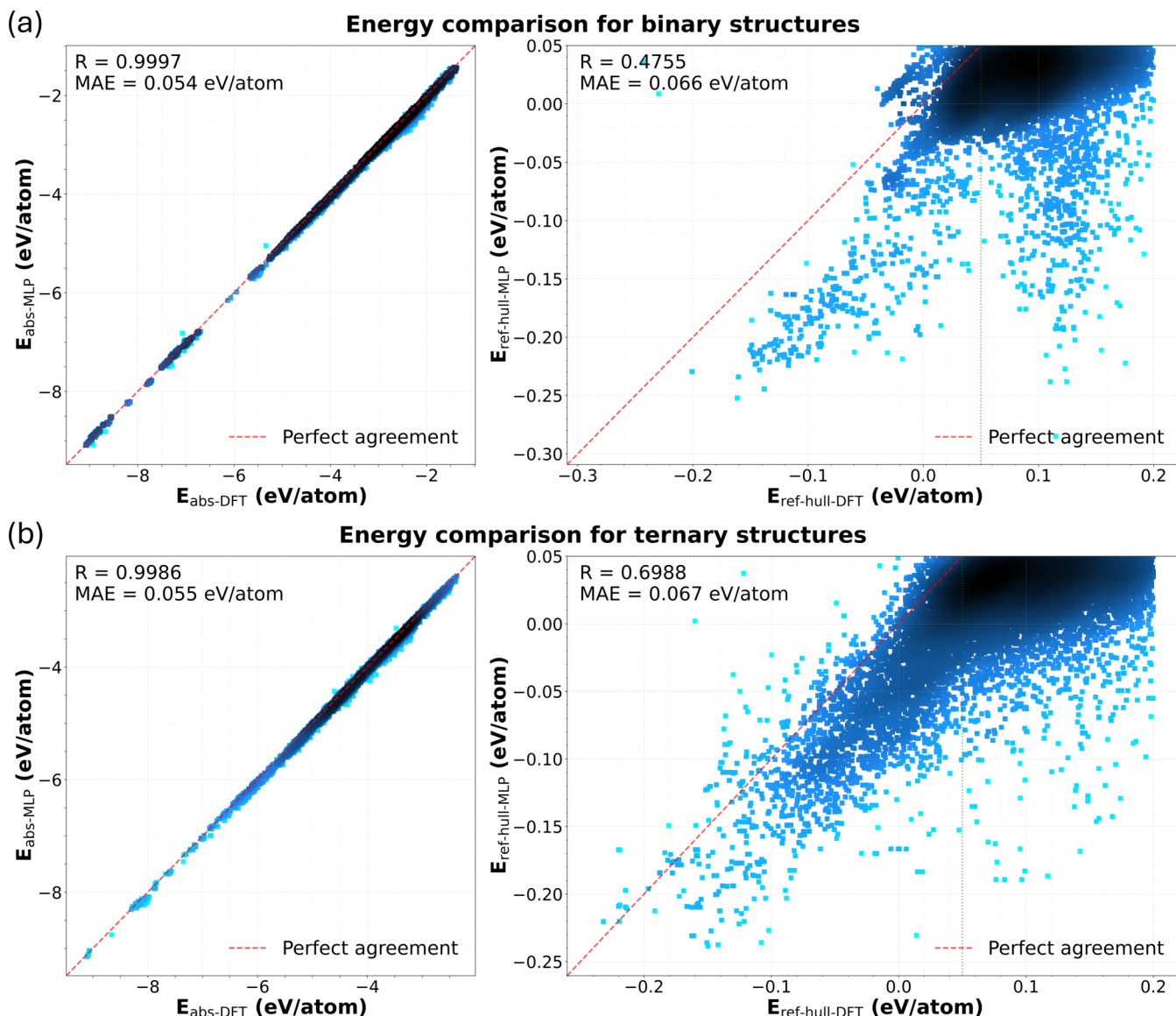


FIG. 2. Validation of MLP energy used in the screening workflow for (a) binary and (b) ternary systems, respectively. In both plots, the left panel shows the comparison in terms of absolute energy per atom (E_{abs}) between MLP and DFT results, while the right panel shows the comparison between energy with respect to the reference convex hull values ($E_{\text{ref-hull}}$) from the available materials project data.

MatterGen and MatterSim are used to rapidly explore and prescreen candidates, achieving significant speedup over conventional DFT approaches. Finally, a two-stage DFT validation protocol further reduces computational costs by avoiding unnecessary calculation on noninteresting structures. This workflow efficiently identifies promising electrider candidates across vast chemical space while maintaining rigor necessary for materials discovery.

III. RESULTS AND DISCUSSIONS

A. Validation of hierarchical screening workflow

As illustrated in Fig. 1, the workflow reduces the candidate pool from 79 244 to 17 195 for binary and from 285 120 to 18 705 for ternary systems after the MLP prescreen, and then 232 binary and 32 ternary candidates after DFT calculation. Such progressive pruning is expected, since electrider forma-

tion is intrinsically rare. Hence, most generated electron-rich structures either are thermodynamically unfavorable or lack significant interstitial electron localization. In this workflow, the most critical assumption is that our MLP prescreen can effectively discard unstable structures while preserving the vast majority of genuinely promising candidates for the subsequent, more expensive DFT validation.

To verify the MLP accuracy, we compared both absolute energy E_{abs} and $E_{\text{ref-hull}}$ values from MatterSim-MLP and PBE-DFT in Fig. 2 for 17 195 binary and 18 705 ternary structures generated at stages 2 and 3, respectively. Between MatterSim-MLP and VASP-DFT calculated absolute energy values for both binary and ternary compounds, Fig. 2 demonstrates the calculated metrics: Mean absolute errors (MAEs) of 0.054/0.055 eV/atom and correlation coefficient $R = 0.9997/0.9986$ for binary and ternary compounds are consistent with the report as found in the original literature

[47]. The ternary system yields slightly bigger errors, which is expected due to the nature of MLP model construction.

Compared to E_{abs} , E_{hull} is more important in our materials filtering strategy to determine whether a material is energetically favorable. While many metastable structures can exist, it is generally considered that $E_{\text{hull}} < 0.10$ eV/atom is necessary for most compounds, except nitrides [63]. Different from E_{abs} , E_{hull} is a relative quantity with respect to the reference systems, and thus it is more numerically sensitive. According to Fig. 2, the comparison of $E_{\text{ref-hull}}$ values yields similar MAE metrics (0.066 eV/atom for binaries and 0.067 eV/atom for ternaries), while the correlation R value is much smaller (0.4755 for binary and 0.6988 for ternary). Although the correlation is not ideal, it is generally found that MatterSim tends to underestimate, rather than overestimate, the E_{hull} values as compared to the DFT reference. Hence, the MLP prescreen may still consider a fraction of energetically unfavorable structures, but is less likely to miss the vast majority of truly low-energy candidates ($E_{\text{ref-hull-DFT}} < 0.05$ eV/atom), within the 0.10 eV/atom threshold value. Despite the underestimation issue, the use of MLP can effectively prerelax the structure and filter approximately 60% of unstable structures before more expensive VASP calculations, thus saving computational time in our screening framework.

B. Binary electride discovery

Among the screened 1510 binary compositions, we have identified 232 low-energy candidates with $E_{\text{hull-DFT}} < 0.05$ eV/atom (see Figs. S1–S4 in the Supplemental Material [64]). Below, we will briefly showcase the discoveries on two representative systems.

The Ca-P binary was reported to have three stable non-electride phases in the Materials Project, including Ca_5P_8 ($C2/m$: 12), CaP ($P6_2m$: 189) and CaP_3 ($P\bar{1}$: 2). As shown in Fig. 3(a), our search supplements three new candidates with $E_{\text{ref-hull-DFT}} < 0.10$ eV/atom. Remarkably, we identify one new stable phase that was absent from the MP database: $\text{mS32-Ca}_5\text{P}_3$ ($C2/m$: 12), lying 0.205 eV/atom below the original convex hull. This structure is closely related to the well-known $1\text{D-Mn}_5\text{Si}_3$ type [21], but crystallizes in a lower subgroup with the monoclinic symmetry. In addition, two metastable candidates were found to have $E_{\text{hull-DFT}} < 0.10$ eV/atom in the updated convex hull. In particular, the $\text{oS16-Ca}_3\text{P}$ structure ($Cmma$: 65) is an electride with 0.077 eV/atom above the hull. Unlike Ca_5P_3 , the $\text{oS16-Ca}_3\text{P}$ forms a 2D corrugated interstitial electron distribution, suggesting a versatile electride chemistry in this system.

Additionally, we identified a dozen chemical systems exhibiting numerous low-energy structures clustered within electron-rich compositional regions. The Y-N system, shown in Fig. 3(b), exemplifies particularly rich phase behavior, with seven candidates concentrated within a narrow energy range of $E_{\text{hull-DFT}} \leq 0.02$ eV/atom. Notably, one new thermodynamically stable phase, $\text{hR51-Y}_9\text{N}_8$ ($R\bar{3}$: 148), lies 0.036 eV/atom below the original Materials Project convex hull. This $\text{hR51-Y}_9\text{N}_8$ structure is characterized by nitrogen vacancies compared to the stoichiometric YN compound. Between Y and Y_9N_8 , six additional metastable candidates cluster within 0.02 eV/atom of the hull, including multiple Y_8N_7

and Y_4N_3 layered phases ($R\bar{3}m$: 166). These results collectively suggest a thermodynamical route to achieve interstitial electron localization around Y by engineering the nitrogen vacancies in the existing YN compounds.

C. Ternary electride discovery

Extending from binary AB to ternary $AA'B$ compositions ($A' = \text{Al, Si, Ge, Ga, Sn}$) identified 32 low-energy electride candidates with $E_{\text{hull-DFT}} < 0.05$ eV/atom (see details in Figs. S5 and S6 in the Supplemental Material [64]). The small number is expected since our target compositions are slightly apart from the ideal stoichiometry. Hence, most of these compounds are unlikely to be energetically favorable unless the electride phases are formed. Below, we highlight discoveries in two representative systems.

According to Materials Project, the Cs-Al-P system contains only one stable ternary phase: Cs_3AlP_2 . Our results demonstrate that $\text{tP11-Cs}_4\text{Al}_3\text{P}_4$ ($P\bar{4}2m$: 111), with one excess electron per formula unit, is also thermodynamically stable with respect to the existing compounds, with $E_{\text{ref-hull-DFT}} = -0.004$ eV/atom. Figure 4(a) shows the updated ternary phase diagram incorporating $\text{tP11-Cs}_4\text{Al}_3\text{P}_4$. From the diagram, $\text{tP11-Cs}_4\text{Al}_3\text{P}_4$ lies close to the compositional path between the two stoichiometric compounds Cs_3AlP_2 and AlP . Examination of the crystal structure reveals a layered packing with each layer terminated by the electron-positive Cs atoms on both sides. Consequently, it is expected that the excess electron localization between layers stabilizes this composition, similar to the behavior observed in 2D Ca_2N -type electrides. In addition to $\text{tP11-Cs}_4\text{Al}_3\text{P}_4$, we have found a total of six metastable (within 0.05 eV/atom E_{hull}) layered ternary electride candidates across a range of systems, suggesting a rich opportunity to achieving layered electrides in multicomposition compounds.

Our search not only discovers new materials in the underexplored systems, but also uncovers previously overlooked phases. The K-B-O system has been extensively studied due to its technological importance in lubricants and anticorrosion applications, evidenced by the existence of 12 ternary entries in the Materials Project. However, our screening identified one new stable ternary electride: $\text{hP11-K}_6\text{BO}_4$ ($P3$: 143) with $E_{\text{ref-hull-DFT}} = -0.025$ eV/atom [see Fig. 4(b)]. This structure possesses the 1D cavities surrounded by potassium atoms, naturally providing a favorable environment for electron localization. This example demonstrates that generative approaches can identify overlooked compositions even in the extensively studied chemical systems.

D. Electronic structure analysis

Among the 264 identified low-energy electrides, we have found 13 thermodynamically stable electrides, 12 of which exhibit nonimaginary phonon frequencies (see Figs. S7–S11 in the Supplemental Material [64]), suggesting dynamical stability and favorable potential synthetic accessibility. In Fig. 5, we examine the electronic structures of two representative stable ternary electrides, $\text{hP11-K}_6\text{BO}_4$ ($P3$: 143) and $\text{mS26-Cs}_6\text{Al}_2\text{S}_5$ (Cm : 8), which feature different excess electron counts.

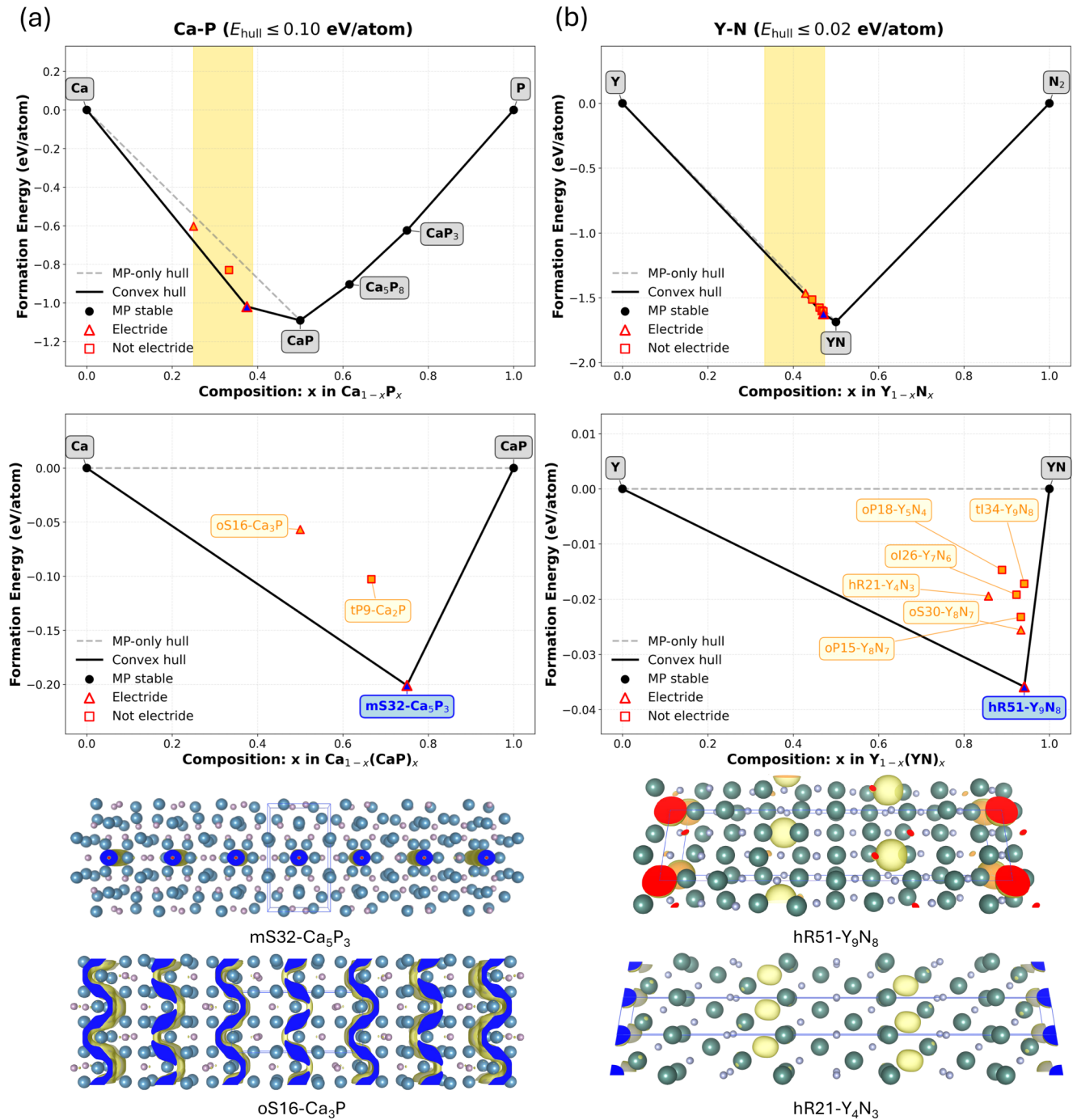


FIG. 3. Convex hulls and new phases for (a) Ca-P and (b) Y-N systems. Top panels show the Materials Project (black circles) and newly discovered phases (red triangles for electriles and red squares for nonelectriles; on-hull structures are filled with blue, above hull structures are filled with orange), with the gray dashed line indicating the original convex hull and the solid black line representing the refined convex hull. The electron-rich compositions with $0 < N_{\text{excess}} \leq 4$ are highlighted in yellow rectangles. The middle panels display an enlarged subconvex hull plot between the elemental metal and the stoichiometric binary with the most negative formation energy. The bottom panels illustrate representative structures from each system with atomic colors: Ca (steel blue), P (pale purple), Y (dark green), and N (light blue); yellow isosurfaces represent excess electrons' distributions.

Figure 5(a) presents the electronic band structure and atom-projected density of states for hP11-K₆BO₄. Given one excess electron per primitive unit cell exists in this compound, we expect the excess electron to partially occupy the highest valence band if electrile formation occurs. Indeed, the band structure, shown in the left panel of Fig. 5(a), exhibits a

characteristic half-filled top valence band. The PDOS analysis (middle panel) reveals that this valence band has negligible projections onto K, B, or O atomic orbitals, demonstrating typical interstitial electron character. The computed partial charge density for the top valence band (right panel) displays a spherical distribution centered at the hexagonal lattice origin

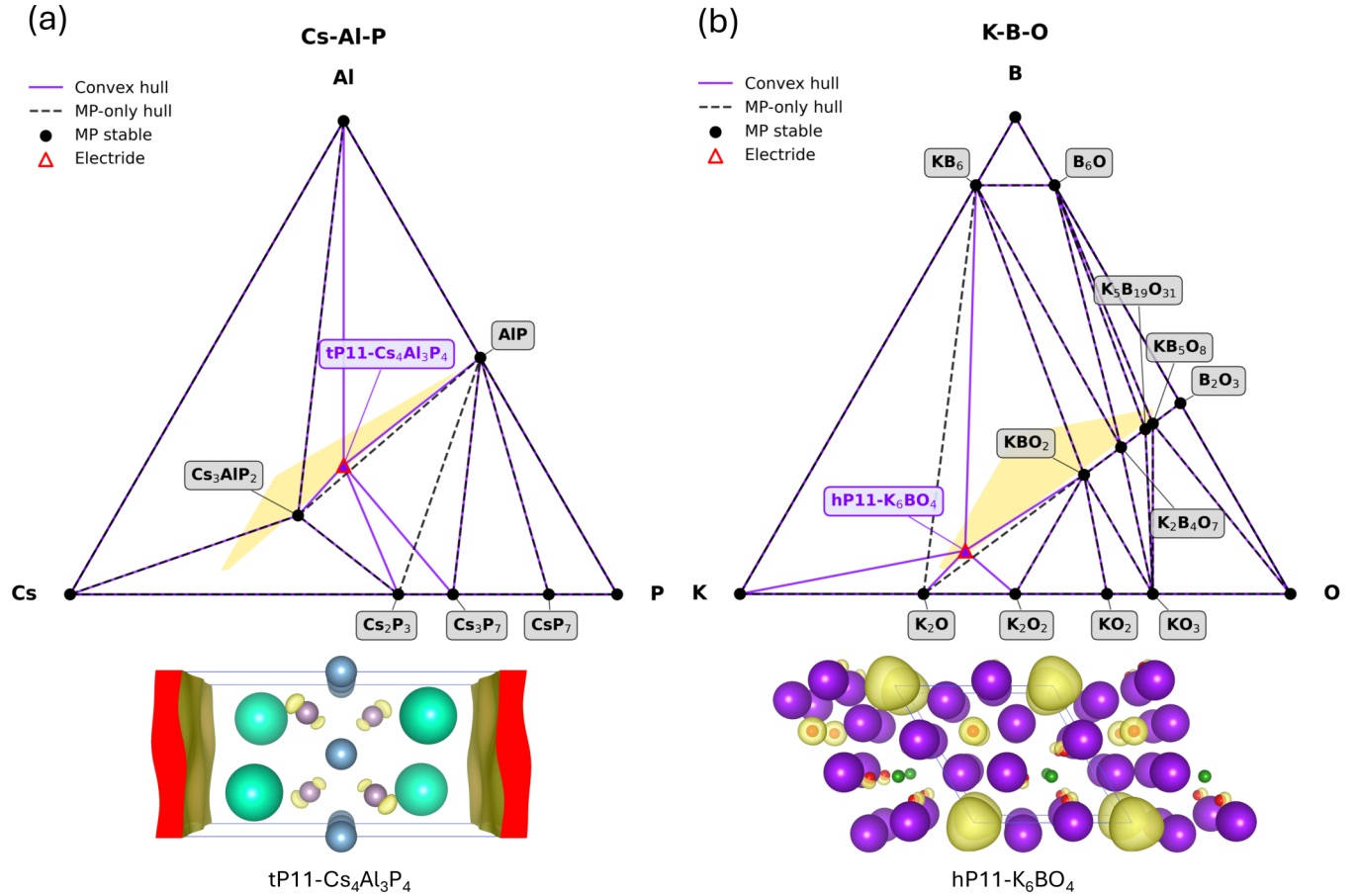


FIG. 4. Ternary convex hulls and new phases for (a) Cs-Al-P and (b) K-B-O systems. Top panels: Dashed black lines indicate original convex hull boundaries; solid purple lines show updated convex hulls after incorporating newly identified electride compounds. Black circles represent Materials Project phases; red triangles denote electride candidates (stable ones are filled with purple). The electron-rich composition region ($0 < N_{\text{excess}} \leq 2$) is highlighted by yellow shading. Bottom panels: Representative electride structures from each system with atomic colors: K (purple), Cs (cyan), Al (gray), B (green), O (red), and P (pale purple); yellow isosurfaces represent excess electrons' distributions. For these two specific ternary systems, there are no metastable candidates that fall within the $E_{\text{hull}} < 0.05$ eV/atom discovery threshold. The complete set of generated electride candidates, including the metastable ones within the discovery threshold for all 15 ternary systems, is provided in Figs. S5 and S6 of the Supplemental Material [64].

(0, 0, 0), consistent with nearly free electron behavior. This interpretation is further supported by the parabolic band dispersion near the Γ point, characteristic of a quasifree electron gas similar to previously identified switchable 2D electrides [65]. In contrast, the second-highest valence band is primarily composed of oxygen's p orbitals, positioned approximately 0.75 eV below the interstitial band, indicating clear electronic separation between interstitial and atomiclike states.

If one excess electron leads to a half-filled interstitial band, one may naturally speculate that two excess electrons result in a fully filled interstitial band. Indeed, the electronic structure of mS26-Cs₆Al₂S₅ in Fig. 5(b) supports this hypothesis. With two excess electrons per primitive unit cell, mS26-Cs₆Al₂S₅ displays a fully filled top valence band, resulting in a semiconducting electride with a PBE band gap of ~ 1.75 eV. However, the PDOS analysis reveals a more nuanced scenario than in hP11-K₆BO₄. The top valence band contains not only interstitial electrons but also notable contributions from sulfur's p orbitals. The partial charge density plot of the top valence band [right panel of Fig. 5(b)] agrees with this observation, showing electron density distributed between

the hexagonal interstitial center and around S atoms. This complex electronic structure arises from the crystal packing, where the structure consists of alternating electron-neutral layers (with five-coordinated Cs) and electron-rich layers (with four-coordinated Cs). Within the electron-rich layers, the undercoordinated Cs atoms form a nearly hexagonal arrangement in-plane, with each Cs donating excess electrons. However, the presence of S and Al atoms causes some electrons to occupy sulfur p orbitals, with the majority localizing at the hexagonal interstitial centers. It is worth noting the interstitial space in mS26-Cs₆Al₂S₅ is more spatially confined due to the existence of in-plane Al and S atoms. If a more spacious interstitial environment were available, one could potentially achieve a fully interstitial-character valence band without PDOS on the atomic sites. That said, mS26-Cs₆Al₂S₅ still exhibits clear electride character, as confirmed by the significant interstitial electron localization at the top valence band. Similar to hP11-K₆BO₄, the second-highest valence band is composed on sulfur's p orbitals with about 1.0 eV separation from the top valence band. This plot is not shown here to maintain the clarity.

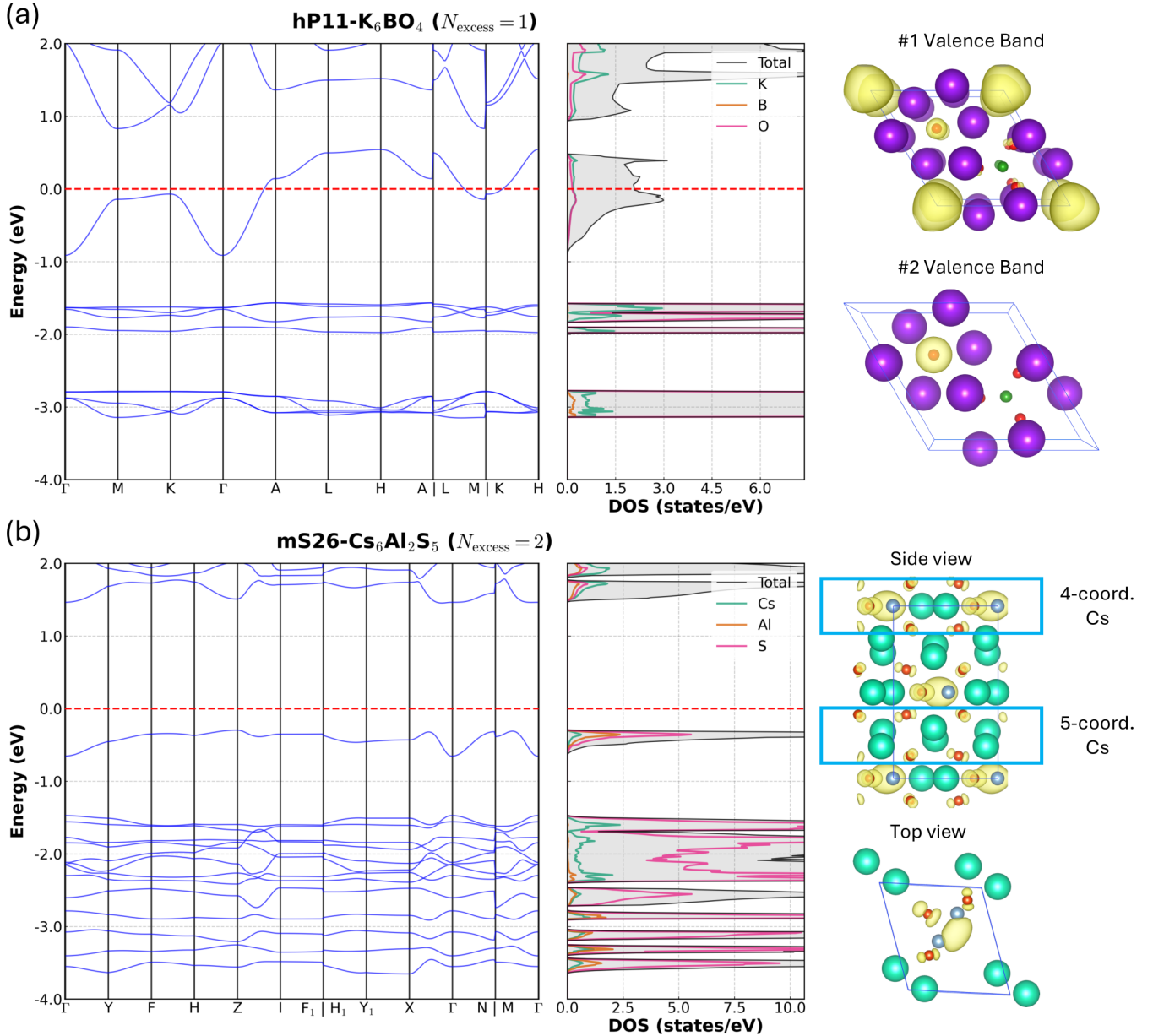


FIG. 5. Electronic structures of two representative stable ternary electrider compounds: (a) hP11-K₆BO₄ and (b) mS26-Cs₆Al₂S₅. Left panels: Band structures and projected density of states (PDOS). Right panels: Partial charge density distributions for the top valence bands in hP11-K₆BO₄ and mS26-Cs₆Al₂S₅ (shown in top and side views). Atomic colors: K (purple), Cs (cyan), Al (gray), B (green), O (red), and S (orange); yellow isosurfaces represent the electron charge density.

In our screening, most electrider compounds exhibit $N_{\text{excess}} = 1$, corresponding to a half-filled top valence band, consistent with the majority of previously identified electrider compounds. This observation suggests two complementary avenues for future exploration. First, restricting the target composition space to lower N_{excess} values could enable more efficient systematic exploration of extended chemical spaces beyond ternary compositions. Second, screening compositions with $N_{\text{excess}} = 2$ offers greater likelihood for identifying intrinsically semiconducting electrider compounds with enhanced thermodynamic stability for applications in semiconducting devices. These insights point toward more targeted screening strategies for expanding the electrider materials landscape.

IV. CONCLUSION

In this work, we have presented an accelerated framework for inorganic electrider discovery by integrating physical principles, generative AI, ML potentials, and high-throughput DFT validation. Compared to the traditional framework based on DFT calculations, our approach can efficiently explore vast chemical space with significantly reduced computational costs, while maintaining the necessary accuracy. Using this workflow on a targeted chemical space of electron-rich binary and ternary compositions, we have identified 264 new electrider candidates within 0.05 eV/atom above the convex hull, substantially expanding the known electrider landscape.

We highlight the following key components in our work.

First, chemical space selection based on physical principles is essential for efficient materials discovery. Rather than uniformly exploring all possible compositions, restricting the search to electron-rich systems with electropositive metals dramatically reduces combinatorial complexity while maintaining access to chemically reasonable candidates without sacrificing discovery potential.

Second, the use of MatterGen and MatterSim allows rapid generation and screening of low-energy structures across thousands of compositions. This approach achieves a significant speedup to enable systematic exploration of chemical space previously inaccessible to computational materials discovery.

Third, the identification of new stable phases demonstrates that generative methods can uncover compositional variants and structural prototypes overlooked by previous database-mining approaches, suggesting substantial opportunities for targeted re-examination of existing materials spaces.

Finally, these discoveries underscore the transformative potential of modern AI and ML tools in materials discovery. However, it is critical to acknowledge that both MatterGen and MatterSim were trained on existing data, which may introduce biases toward chemically conventional compositions and known structural families. Future work should explore training generative models on more diverse datasets.

Our framework combining physical insights, generative modeling, and ML prescreening provides a roadmap for accelerated discovery across diverse functional materials beyond electrides, establishing a new paradigm for materials exploration in the age of AI-driven science. Transferring the workflow to a new target requires adapting mainly two components: (1) a composition-level physical descriptor that

constrains the chemical space (analogous to the excess-electron count used here) and (2) a property analyzer applied in the final high-throughput DFT stage; the generative sampling, ML-potential prescreening, and hierarchical DFT validation can be reused. With these minimal changes, the same pipeline can be applied to, for example, thermoelectrics (screening for low lattice thermal conductivity or favorable power factor) [51–53], conventional superconductors (electron-phonon coupling, to which the free-electron-like states of electrides are themselves germane) [22,66], topological semimetals and insulators (band-inversion descriptors, again naturally connected to weakly bound interstitial electrons) [24–26,67], low-work-function electron emitters [12], catalysts [9,11], and magnetic materials [43]. The identified candidates may stimulate further experimental efforts to assess their practical utility for applications.

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All authors declare that they have no conflict of interest.

DATA AVAILABILITY

The source code, instructions, and scripts used to calculate the results of this study are available in Ref. [68]. The newly identified electrides are also interactively available via Ref. [69].

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- [1] J. L. Dye, Electrides: Ionic salts with electrons as the anions, *Science* **247**, 663 (1990).
 - [2] J. L. Dye, Electrides: Early examples of quantum confinement, *Acc. Chem. Res.* **42**, 1564 (2009).
 - [3] S. B. Dawes, D. L. Ward, R. H. Huang, and J. L. Dye, First electride crystal structure, *J. Am. Chem. Soc.* **108**, 3534 (1986).
 - [4] H. Hosono and M. Kitano, Advances in materials and applications of inorganic electrides, *Chem. Rev.* **121**, 3121 (2021).
 - [5] R. H. Huang, M. K. Faber, K. J. Moeggenborg, D. L. Ward, and J. L. Dye, Structure of K^+ (cryptand[2.2.2]) electride and evidence for trapped electron pairs, *Nature (London)* **331**, 599 (1988).
 - [6] D. J. Singh, H. Krakauer, C. Haas, and W. E. Pickett, Theoretical determination that electrons act as anions in the electride $Cs^+(15\text{-crown-5})_2 \cdot e^-$, *Nature (London)* **365**, 39 (1993).
 - [7] L. D. Le, D. Issa, B. Van Eck, and J. L. Dye, Preparation of alkali and electride films by direct vapor deposition, *J. Phys. Chem.* **86**, 7 (1982).
 - [8] S. Matsuishi, Y. Toda, M. Miyakawa, K. Hayashi, T. Kamiya, M. Hirano, I. Tanaka, and H. Hosono, High-density electron anions in a nanoporous single crystal: $[Ca_{24}Al_{28}O_{64}]^{4+}(4e^-)$, *Science* **301**, 626 (2003).
 - [9] M. Kitano, Y. Inoue, Y. Yamazaki, F. Hayashi, S. Kanbara, S. Matsuishi, T. Yokoyama, S.-W. Kim, M. Hara, and H. Hosono, Ammonia synthesis using a stable electride as an electron donor and reversible hydrogen store, *Nat. Chem.* **4**, 934 (2012).
 - [10] S. Kanbara, M. Kitano, Y. Inoue, T. Yokoyama, M. Hara, and H. Hosono, Mechanism switching of ammonia synthesis over Ru-loaded electride catalyst at metal–insulator transition, *J. Am. Chem. Soc.* **137**, 14517 (2015).
 - [11] M. Kitano, S. Kanbara, Y. Inoue, N. Kuganathan, P. V. Sushko, T. Yokoyama, M. Hara, and H. Hosono, Electride support boosts nitrogen dissociation over ruthenium catalyst and shifts the bottleneck in ammonia synthesis, *Nat. Commun.* **6**, 6731 (2015).
 - [12] C. Drobny, K. Wätzig, A. Rost, and M. Tajmar, Endurance operation of a heaterless C12A7 electride plasma cathode and post operation material analysis, *Acta Astronaut.* **214**, 231 (2024).
 - [13] S. Zhao, E. Kan, and Z. Li, Electride: From computational characterization to theoretical design, *WIREs Comput. Mol. Sci.* **6**, 430 (2016).
 - [14] C. Liu, S. A. Nikolaev, W. Ren, and L. A. Burton, Electrides: A review, *J. Mater. Chem. C* **8**, 10551 (2020).
 - [15] K. Lee, S. W. Kim, Y. Toda, S. Matsuishi, and H. Hosono, Dicalcium nitride as a two-dimensional electride with an anionic electron layer, *Nature (London)* **494**, 336 (2013).
 - [16] D. L. Druffel, K. L. Kuntz, A. H. Woomer, F. M. Alcorn, J. Hu, C. L. Donley, and S. C. Warren, Experimental demonstration of

- an electride as a 2D material, *J. Am. Chem. Soc.* **138**, 16089 (2016).
- [17] T. Tada, S. Takemoto, S. Matsuishi, and H. Hosono, High-throughput *ab initio* screening for two-dimensional electride materials, *Inorg. Chem.* **53**, 10347 (2014).
- [18] W. Ming, M. Yoon, M.-H. Du, K. Lee, and S. W. Kim, First-principles prediction of thermodynamically stable two-dimensional electrides, *J. Am. Chem. Soc.* **138**, 15336 (2016).
- [19] Y. Zhang, H. Wang, Y. Wang, L. Zhang, and Y. Ma, Computer-assisted inverse design of inorganic electrides, *Phys. Rev. X* **7**, 011017 (2017).
- [20] J. Wang, K. Hanzawa, H. Hiramatsu, J. Kim, N. Umezawa, K. Iwanaka, T. Tada, and H. Hosono, Exploration of stable strontium phosphide-based electrides: Theoretical structure prediction and experimental validation, *J. Am. Chem. Soc.* **139**, 15668 (2017).
- [21] Y. Lu, J. Li, T. Tada, Y. Toda, S. Ueda, T. Yokoyama, M. Kitano, and H. Hosono, Water durable electride Y_3Si_3 : Electronic structure and catalytic activity for ammonia synthesis, *J. Am. Chem. Soc.* **138**, 3970 (2016).
- [22] Y. Zhang, B. Wang, Z. Xiao, Y. Lu, T. Kamiya, Y. Uwatoko, H. Kageyama, and H. Hosono, Electride and superconductivity behaviors in Mn_5Si_3 -type intermetallics, *npj Quantum Mater.* **2**, 45 (2017).
- [23] Y. Zhang, Z. Xiao, T. Kamiya, and H. Hosono, Electron confinement in channel spaces for one-dimensional electride, *J. Phys. Chem. Lett.* **6**, 4966 (2015).
- [24] M. Hirayama, S. Matsuishi, H. Hosono, and S. Murakami, Electrides as a new platform of topological materials, *Phys. Rev. X* **8**, 031067 (2018).
- [25] C. Park, S. W. Kim, and M. Yoon, First-principles prediction of new electrides with nontrivial band topology based on one-dimensional building blocks, *Phys. Rev. Lett.* **120**, 026401 (2018).
- [26] H. Huang, K.-H. Jin, S. Zhang, and F. Liu, Topological electride Y_2C , *Nano Lett.* **18**, 1972 (2018).
- [27] Y. Ma, M. Eremets, A. R. Oganov, Y. Xie, I. Trojan, S. Medvedev, A. O. Lyakhov, M. Valle, and V. Prakapenka, Transparent dense sodium, *Nature (London)* **458**, 182 (2009).
- [28] M.-S. Miao and R. Hoffmann, High pressure electrides: A predictive chemical and physical theory, *Acc. Chem. Res.* **47**, 1311 (2014).
- [29] M.-S. Miao and R. Hoffmann, High-pressure electrides: The chemical nature of interstitial quasiatoms, *J. Am. Chem. Soc.* **137**, 3631 (2015).
- [30] B. Wan, J. Zhang, L. Wu, and H. Gou, High-pressure electrides: From design to synthesis, *Chin. Phys. B* **28**, 106201 (2019).
- [31] I. I. Naumov and R. J. Hemley, Metallic surface states in elemental electrides, *Phys. Rev. B* **96**, 035421 (2017).
- [32] L. A. Burton, F. Ricci, W. Chen, G.-M. Rignanese, and G. Hautier, High-throughput identification of electrides from all known inorganic materials, *Chem. Mater.* **30**, 7521 (2018).
- [33] J. Zhou, L. Shen, M. Yang, H. Cheng, W. Kong, and Y. P. Feng, Discovery of hidden classes of layered electrides by extensive high-throughput material screening, *Chem. Mater.* **31**, 1860 (2019).
- [34] Q. Zhu, T. Frolov, and K. Choudhary, Computational discovery of inorganic electrides from an automated screening, *Matter* **1**, 1293 (2019).
- [35] J. Wang, Q. Zhu, Z. Wang, and H. Hosono, Ternary inorganic electrides with mixed bonding, *Phys. Rev. B* **99**, 064104 (2019).
- [36] T. Inoshita, S. Jeong, N. Hamada, and H. Hosono, Exploration for two-dimensional electrides via database screening and *ab initio* calculation, *Phys. Rev. X* **4**, 031023 (2014).
- [37] L. M. McRae, R. C. Radomsky, J. T. Pawlik, D. L. Druffel, J. D. Sundberg, M. G. Lanetti, C. L. Donley, K. L. White, and S. C. Warren, Sc_2C , a 2D semiconducting electride, *J. Am. Chem. Soc.* **144**, 10862 (2022).
- [38] B. Kang, K. Parrish, and Q. Zhu, First-principles investigation of electrides derived from sodalites, *J. Phys. Chem. C* **127**, 18745 (2023).
- [39] C. Liu, M. M. Mukta, B. Kang, and Q. Zhu, Semiconducting electrides derived from sodalite: A first-principles study, *ACS Omega* **10**, 1635 (2025).
- [40] S.-C. Zhu, L. Wang, J.-Y. Qu, J.-J. Wang, T. Frolov, X.-Q. Chen, and Q. Zhu, Computational design of flexible electrides with nontrivial band topology, *Phys. Rev. Mater.* **3**, 024205 (2019).
- [41] P. Chanhom, K. E. Fritz, L. A. Burton, J. Kloppenburg, Y. Filinchuk, A. Senyshyn, M. Wang, Z. Feng, N. Insin, J. Suntivich, *et al.*, Sr_3CrN_3 : A new electride with a partially filled *d*-shell transition metal, *J. Am. Chem. Soc.* **141**, 10595 (2019).
- [42] A. Merchant, S. Batzner, S. S. Schoenholz, M. Aykol, G. Cheon, and E. D. Cubuk, Scaling deep learning for materials discovery, *Nature (London)* **624**, 80 (2023).
- [43] C. Zeni, R. Pinsler, D. Zügner, A. Fowler, M. Horton, X. Fu, Z. Wang, A. Shysheya, J. Crabbé, S. Ueda, *et al.*, A generative model for inorganic materials design, *Nature (London)* **639**, 624 (2025).
- [44] R. Jiao, W. Huang, P. Lin, J. Han, P. Chen, Y. Lu, and Y. Liu, in *Advances in Neural Information Processing Systems*, edited by A. Oh, T. Naumann, A. Globerson, K. Saenko, M. Hardt, and S. Levine (Curran Associates, Inc., Red Hook, NY, USA, 2023), Vol. 36, pp. 17464–17497.
- [45] D. Levy, S. S. Panigrahi, S.-O. Kaba, Q. Zhu, M. Galkin, S. Miret, and S. Ravanbakhsh, in *AI for Accelerated Materials Design Workshop at NeurIPS 2024* (Vancouver, BC, Canada, 2024).
- [46] B. K. Miller, R. T. Q. Chen, A. Sriram, and B. M. Wood, in *Proceedings of the 41st International Conference on Machine Learning*, edited by R. Salakhutdinov, Z. Kolter, K. Heller, A. Weller, N. Oliver, J. Scarlett, and F. Berkenkamp (PMLR, Vienna, Austria, 2024), Vol. 235, pp. 35664–35686.
- [47] H. Yang, C. Hu, Y. Zhou, X. Liu, Y. Shi, J. Li, G. Li, Z. Chen, S. Chen, C. Zeni, *et al.*, MatterSim: A deep learning atomistic model across elements, temperatures and pressures, *arXiv:2405.04967*.
- [48] I. Batatia, P. Benner, Y. Chiang, A. M. Elena, D. P. Kovács, J. Riebesell, X. R. Advincula, M. Asta, M. Avaylon, W. J. Baldwin, *et al.*, A foundation model for atomistic materials chemistry, *J. Chem. Phys.* **163**, 184110 (2025).
- [49] B. M. Wood, M. Dzamba, X. Fu, M. Gao, M. Shuaibi, L. Barroso-Luque, K. Abdelmaqsoud, V. Gharakhanyan, J. R. Kitchin, D. S. Levine, *et al.*, UMA: A family of universal models for atoms, *arXiv:2506.23971*.
- [50] A. K. Cheetham and R. Seshadri, Artificial intelligence driving materials discovery? Perspective on the article: Scaling deep learning for materials discovery, *Chem. Mater.* **36**, 3490 (2024).

- [51] A. Ghafarollahi and M. J. Buehler, Autonomous in-silico inorganic materials discovery via multi-agent physics-aware scientific reasoning, *npj Comput. Mater.* (2026).
- [52] L. Guo, Y. Liu, Z. Chen, H. Yang, D. Donadio, and B. Cao, Generative deep learning for predicting ultrahigh lattice thermal conductivity materials, *npj Comput. Mater.* **11**, 97 (2025).
- [53] Y. Long, C. Zhong, X. Ma, J. Zhang, H. Yao, J. Liu, K. Hu, Q. Zhang, and X. Lin, Inverse design of high-performance thermoelectric materials via a generative model combined with experimental verification, *ACS Appl. Mater. Interfaces* **17**, 19856 (2025).
- [54] X. Dong, A. R. Oganov, H. Cui, X.-F. Zhou, and H.-T. Wang, Electronegativity and chemical hardness of elements under pressure, *Proc. Natl. Acad. Sci. USA* **119**, e2117416119 (2022).
- [55] S. Fredericks, K. Parrish, D. Sayre, and Q. Zhu, PyXtal: A Python library for crystal structure generation and symmetry analysis, *Comput. Phys. Commun.* **261**, 107810 (2021).
- [56] S. P. Ong, W. D. Richards, A. Jain, G. Hautier, M. Kocher, S. Cholia, D. Gunter, V. L. Chevrier, K. A. Persson, and G. Ceder, Python Materials Genomics (pymatgen): A robust, open-source Python library for materials analysis, *Comput. Mater. Sci.* **68**, 314 (2013).
- [57] G. Kresse and J. Furthmüller, Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set, *Phys. Rev. B* **54**, 11169 (1996).
- [58] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [59] P. E. Blöchl, Projector augmented-wave method, *Phys. Rev. B* **50**, 17953 (1994).
- [60] G. Henkelman, A. Arnaldsson, and H. Jonsson, A fast and robust algorithm for Bader decomposition of charge density, *Comput. Mater. Sci.* **36**, 354 (2006).
- [61] A. H. Larsen, J. J. Mortensen, J. Blomqvist, I. E. Castelli, R. Christensen, M. Dułak, J. Friis, M. N. Groves, B. Hammer, C. Hargus, *et al.*, The atomic simulation environment—A Python library for working with atoms, *J. Phys.: Condens. Matter* **29**, 273002 (2017).
- [62] A. Togo, F. Oba, and I. Tanaka, First-principles calculations of the ferroelastic transition between rutile-type and CaCl_2 -type SiO_2 at high pressures, *Phys. Rev. B* **78**, 134106 (2008).
- [63] W. Sun, S. T. Dacek, S. P. Ong, G. Hautier, A. Jain, W. D. Richards, A. C. Gamst, K. A. Persson, and G. Ceder, The thermodynamic scale of inorganic crystalline metastability, *Sci. Adv.* **2**, e1600225 (2016).
- [64] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/cq1m-y96b> for (1) additional convex hull analyses of binary and ternary systems and (2) phonon calculations of selected thermodynamically stable structures that have not been included in the main text.
- [65] X. Yang, K. Parrish, Y.-L. Li, B. Sa, H. Zhan, and Q. Zhu, Switchable two-dimensional electrides: A first-principles study, *Phys. Rev. B* **103**, 125103 (2021).
- [66] X. Zhang, Y. Yao, S. Ding, A. Bergara, F. Li, Y. Liu, X.-F. Zhou, and G. Yang, Superconductivity in Li_8Au electride, *Phys. Rev. B* **107**, L100501 (2023).
- [67] S. Nie, Y. Qian, J. Gao, Z. Fang, H. Weng, and Z. Wang, Application of topological quantum chemistry in electrides, *Phys. Rev. B* **103**, 205133 (2021).
- [68] S. Tao and Q. Zhu, ElectrideFlow—High-throughput inorganic electride discovery workflow accelerated by generative models and hierarchical prescreening, GitHub, 2026, <https://github.com/MaterSim/ElectrideFlow>.
- [69] S. Tao and Q. Zhu, Inorganic Electride Database, 2026, <https://mmi.charlotte.edu/electride>.