

How SISSO-derived materials genes shape materials properties: An analytical sensitivity analysisLucas Foppa^{1,2,*} and Matthias Scheffler¹¹*The NOMAD Laboratory at BIFOLD, Technical University of Berlin, Franklinstr. 28/29, 10587 Berlin, Germany*²*Molecular Simulations from First Principles e.V., Akazienstr. 3A, 10823 Berlin, Germany*

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Interpretable AI can reveal physical principles governing intricate materials properties by uncovering explicit relationships between physical parameters and target properties. The sure-independence screening and sparsifying operator (SISSO) symbolic regression approach identifies analytical expressions that correlate a target property with a small set of parameters, termed *materials genes*, selected from a large pool of candidates. However, multiple gene combinations can yield equally accurate SISSO models, with individual genes contributing with different weights. Here, we establish a derivative-based sensitivity analysis that enhances interpretability, thereby enabling deeper physical insight. This analysis also reveals how distinct gene combinations encode equivalent information and identifies valence orbital radii, nuclear charges, and their products as the key quantities governing the equilibrium lattice constant of perovskites.

DOI: [10.1103/gk23-cfh1](https://doi.org/10.1103/gk23-cfh1)**I. INTRODUCTION**

Predictive models linking basic physical parameters to materials properties and functions are key to accelerating materials discovery. Atomistic simulations accurately predict some materials properties. They offer detailed physical insights, but are inappropriate to model properties governed by multiple entangled physical processes. AI and machine learning reveal, based on appropriate data, nonlinear correlations between multiple input parameters, termed primary features, and target properties [1–4]. These methods might thus capture intricate materials properties more effectively than explicit theoretical approaches. However, their flexibility often comes at the cost of interpretability, as many AI models act as “black boxes,” providing limited insight into the physical mechanisms governing the materials properties. To mitigate this problem, primary-feature-importance analyses are often used to identify the most critical primary features for the models, thereby providing more physical insight. Such explainable AI analyses [5,6] can be based on different concepts such as permutation of primary features [7], local approximations such as the local interpretable model-agnostic explanations (LIME) approach [8], and the SHapley Additive exPlanations (SHAP) method [9–11].

As an alternative to black-box models, symbolic regression (SR) [12–17] has emerged as an approach with the potential to produce interpretable models. SR identifies models for materials properties as analytical expressions, thereby rendering

explicit a mathematical relationship between the primary features and the target materials property of interest. Some SR approaches can also take into account relationships described by derivatives or integrals [18,19]. The sure independence screening and sparsifying operator (SISSO) method [15,20] has gained prominence because of its deterministic and efficient expression-selection process. SISSO has been utilized in a number of applications in materials science [21–25] and catalysis [26–30]. This approach begins by generating an immensity of candidate analytical functions from an initial set of physically meaningful primary features that characterize the material and the environment. These functions are formed by iteratively applying (nonlinear) unary and binary mathematical operators such as addition, multiplication, and logarithm, in order to combine the primary features. Then, compressed sensing [31,32] is used to select a small number (often less than four) of analytical functions that, linearly combined by weighting coefficients, best correlate with the target property. The SISSO models typically depend only on a small number of primary features, selected from the large pool of offered ones. These selected primary features are called *materials genes* [26], in analogy to genes in biology and medicine, in order to emphasize their statistical nature and the concept of *correlations* between these materials genes and the property of interest, as opposed to physical laws. The different genes selected in the SISSO models might impact the property to different extents. Additionally, multiple gene combinations can yield equally accurate SISSO models. Thus, the set of genes required to describe a given materials property is not unique. This hinders deeper physical insights and the decision on what additional data needs to be acquired for accurately modeling the materials property of interest.

One strategy used by some authors to obtain SISSO models that depend only on the few most important primary features has been to evaluate the correlations between primary features and exclude primary features that are highly correlated

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with other primary features before model training [33,34]. However, important correlations, e.g., resulting from the interaction of multiple primary features, i.e., the combination of two primary features according to a binary operator such as difference, might be missed when correlated primary features are excluded prior to model training. Thus, in this paper, we emphasize that sensitivity analyses may be preferable to identify the most influential primary features *after* a model is obtained based on a comprehensive set of primary features [20,35–38].

Sensitivity analyses examine how changes in an (input) primary feature affect the model target-property description (output). They can provide *local* sensitivity scores per data point, e.g., per material, or *global* sensitivity scores averaged over all materials in a dataset. The Sobol method, for instance, is a global sensitivity analysis [20,36,39] that quantifies how much each primary feature contributes to the variance of the model output. It does so by systematically varying the input primary features and decomposing the resulting output variance into contributions from individual primary features as well as their interactions. The resulting Sobol indices provide an interpretable measure of the relative importance of each primary feature and primary-feature combination for the model.

Here, we establish a gradient-based partial-effects (PE) sensitivity analysis to enhance interpretability, enabling deeper physical insight. The PE method [40,41] quantifies the impact of a given primary feature in the model's output by means of the partial derivatives [41,42]. Thus, PE quantifies the weight of a primary feature when the remaining primary features are kept unchanged. PEs provide global as well as local sensitivity scores and the analysis is less computationally demanding than other widely used ones, as, for SISO, the partial derivatives are obtained analytically. PEs recover feature importance scores [41], and this approach has been previously applied to analyze models derived by genetic-algorithm-based SR methods [41,42]. The novelty of this work is the application of the PE approach to models of materials properties identified by the compressed-sensing-based symbolic-regression SISO method.

II. RESULTS AND DISCUSSION

A. SISO model

As an example, we demonstrate the power of the PE analysis for the SISO modeling of the equilibrium lattice constant (a_0) of cubic $A_2BB'O_6$ double perovskites. Obviously, the concept also works for any other materials property and any other class of materials. It has also been employed for a study in heterogeneous catalysis [30]. In the perovskite formula, we define B' as the more electronegative element than B . Single perovskites with the formula ABO_3 (with $B = B'$) are also included in the dataset of 4,583 compounds. The target a_0 was calculated using density functional theory (DFT) with the PBEsol [43] exchange-correlation functional and the FHI-aims code [44,45]. As primary features, we offer 23 basic physical parameters. These include properties of free-atoms of the elements A , B , and B' evaluated with DFT-PBEsol, such as, for example, the radii of s and valence (val) orbitals of the

neutral and +1 cation (cat) of free atoms (r_s , r_{val} , r_s^{cat} , and $r_{\text{val}}^{\text{cat}}$), the electron affinity (EA), and the ionization potential (IP). EA and IP are calculated by the total energy difference between the neutral and charged atoms. The oxidation states of A and the average oxidation state of B and B' elements in the perovskite composition (n_A and $n_{\bar{B}}$), approximated by integers determined based on the periodic table group of A and charge neutrality of the formula unit, are also included. Note that the charge neutrality condition results in the relation $n_A + n_{\bar{B}} = 6$. Some of the primary features are correlated with each other (see Pearson correlation matrix in the Supplemental Material, SM [46]), but this is not a limitation for SISO. A nested 5-fold cross-validation scheme is used to determine the hyperparameters of the SISO models and to estimate their predictive performance in terms of test (prediction) errors. Details about the SISO method and the dataset are given in the SM [46].

The expression of the SISO model for the equilibrium lattice constant (a_0^{SISO}) with the lowest root mean squared error (RMSE) identified based on the 23 primary features is

$$a_0^{\text{SISO}} = 3.50 + 7.41 \times 10^{-3} d_1 + 2.89 \times 10^{-3} d_2 + 3.01 \times 10^{-3} d_3, \quad (1)$$

where

$$d_1 = (r_{s,B})^6 + (r_{s,B'}^{\text{cat}})^6, \quad (2)$$

$$d_2 = \frac{Z_A}{r_{s,A}} (r_{\text{val},B}^{\text{cat}} + r_{\text{val},A}) \quad (3)$$

$$d_3 = r_{\text{val},B}^{\text{cat}} Z_B + r_{\text{val},B'}^{\text{cat}} Z_{B'}. \quad (4)$$

The training R^2 and RMSE are 0.868 and 0.048 Å, respectively, while the test R^2 and RMSE are 0.853 and 0.051 Å, respectively. In Eqs. (2)–(4), Z_A , Z_B , and $Z_{B'}$ are the nuclear charges of elements A , B and B' , $r_{s,A}$ and $r_{\text{val},A}$ are the radii of the s and valence orbitals of the A neutral atom, $r_{s,B}$ is the radius of the s orbital of the B neutral atom, $r_{\text{val},B}^{\text{cat}}$ is the radius of the valence orbital of B^{+1} cation, and $r_{s,B'}^{\text{cat}}$ and $r_{\text{val},B'}^{\text{cat}}$ are the radii of the s and valence orbitals of the B'^{+1} cation. Before discussing the PE approach, let us analyze the materials-property map provided by the SISO model of Eq. (1).

A three-dimensional materials-property map is created using the analytical functions (or descriptors) d_1 , d_2 , and d_3 [Eqs. (2)–(4)] identified by SISO [Fig. 1(a)]. The color scale in Fig. 1(a) indicates the predicted lattice constant a_0^{SISO} . This map guides the discovery of materials that were not considered in the training set but are part of a broader pool of possible materials—or even the full population. In general, one does not know which points in descriptor space correspond to a material, since, mathematically, the values of the different primary features in the descriptor components might be continuous and depend on each other. Thus, they cannot be arbitrarily chosen. However, the population of single and double perovskites is discrete and finite, as it is determined by the periodic table elements that can enter in their compositions. Selecting A elements from alkali, alkaline earth, and scandium groups and B/B' elements from the transition and posttransition metal groups of the periodic table (see the SM

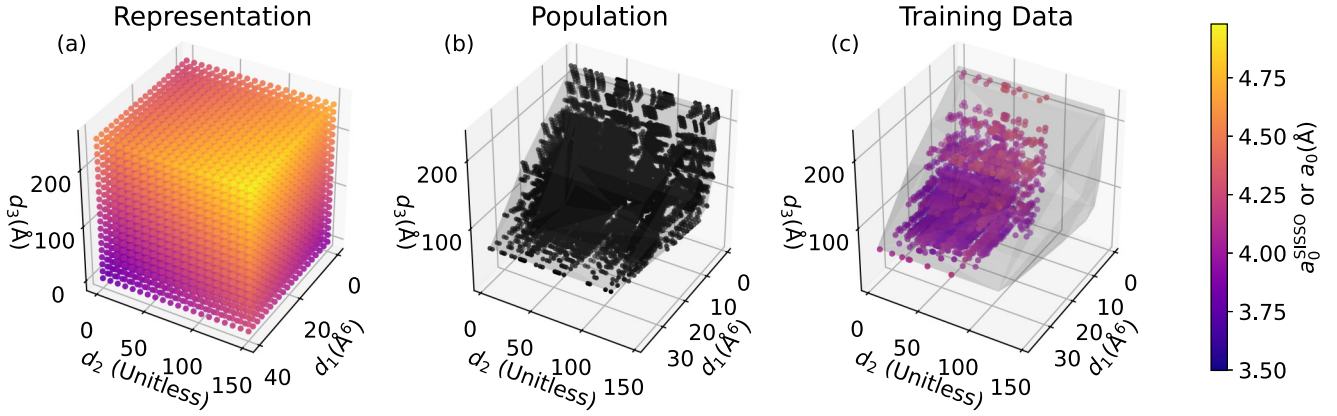


FIG. 1. Three-dimensional materials-property map as defined by the SISSO model for the equilibrium lattice constant of cubic $A_2BB'O_6$ perovskites [a_0^{SISSO} , Eq. (1)]. The map coordinates d_1 , d_2 , and d_3 are the analytical functions shown in Eqs. (2)–(4). The color scale in (a) indicates the predictions of the model a_0^{SISSO} . The black circles in (b) correspond to all possible materials in the population. The circles in (c) correspond to the materials in the training data, and they are colored according to their a_0 values calculated by DFT-PBEsol. The gray surfaces in (b) and (c) indicate the convex hull formed by the population.

[46]), we define a population of 22,496 compounds. These compounds are shown as black circles in Fig. 1(b). Some of these materials might not be stable, as indicated (with some probability) by the Goldschmidt tolerance factor [47] and its SISSO-refined form [22]. This explicit enumeration of materials enables us to identify the borders of the space defined by this population, e.g., by the convex hull in descriptor space, shown as gray surfaces in Fig. 1(b). In Fig. 1(c), each circle corresponds to one of the 4,583 materials in the training dataset. The circles are colored according to their a_0 values calculated with DFT-PBEsol. The map of Fig. 1(c) highlights that the training dataset is not independently and identically distributed with respect to the population. The training samples are concentrated close to the origin of the three-dimensional map, in a region corresponding to low a_0 values. Thus, the accuracy of the SISSO description for regions of the materials space that are underrepresented in the training dataset, e.g., associated with high a_0 , is expected to be lower than that for the portion of the map that is well covered by the training data.

B. Partial-effects sensitivity analysis

In the model of Eq. (1), SISSO selects nine from the 23 offered primary features. In order to identify how each of these nine primary features influences the a_0^{SISSO} model, we evaluate the PEs of the model with respect to a given primary feature ϕ_j as the partial derivative, denoted $PE_{\phi_j}^{a_0^{\text{SISSO}}}$. Because a SISSO model is an analytical function, this derivative can be obtained analytically,

$$PE_{\phi_j}^{a_0^{\text{SISSO}}} = \frac{\partial a_0^{\text{SISSO}}}{\partial \phi_j}. \quad (5)$$

The PE of the model a_0^{SISSO} [Eq. (1)] with respect to the primary feature Z_A , for instance, is

$$PE_{Z_A}^{a_0^{\text{SISSO}}} = \frac{\partial a_0^{\text{SISSO}}}{\partial Z_A} = 2.89 \times 10^{-3} \frac{r_{\text{val},B}^{\text{cat}} + r_{\text{val},A}}{r_{s,A}}. \quad (6)$$

To compare PEs among different primary features that have different units and ranges of values, we scale the PEs based on the standard deviation of the distribution of primary-feature values in the dataset,

$$\text{SPE}_{\phi_j}^{a_0^{\text{SISSO}}} = PE_{\phi_j}^{a_0^{\text{SISSO}}} \times \sigma_{\phi_j}. \quad (7)$$

In Eq. (7), σ_{ϕ_j} corresponds to the standard deviation of the distribution of ϕ_j values in the entire population, e.g., of materials. In general, such population of materials is practically infinite. Thus, σ_{ϕ_j} should be carefully approximated based on finite data, as the results of the PE analysis are sensitive to this scaling. In this work, the entire population of single and double perovskites can be enumerated (see above) and σ_{ϕ_j} is taken as the standard deviation of this entire population of 22,496 materials. The resulting quantities are called *scaled partial effects* (SPEs) and denoted $\text{SPE}_{\phi_j}^{a_0^{\text{SISSO}}}$. Unlike PEs, SPEs have the unit of the target property, here Å. For the primary features that do not appear in Eq. (1), $\text{SPE}_{\phi_j}^{a_0^{\text{SISSO}}}$ is zero. SPEs are local scores reflecting the sensitivity of the model to primary features for a specific material.

The $\text{SPE}_{\phi_j}^{a_0^{\text{SISSO}}}$ values corresponding to the nine primary features of Eq. (1) evaluated for all the compounds in the population of double perovskites are shown in Fig. 2(a). In order to obtain a global score, we average the values of SPE across all materials of the dataset. Here, we considered the absolute values of SPEs, so that the final scores can be compared across primary features irrespective of their sign. The global absolute SPEs for the primary features Z_A , Z_B , $Z_{B'}$, $r_{s,A}$, $r_{\text{val},A}$, $r_{s,B}$, $r_{\text{val},B}^{\text{cat}}$, $r_{s,B'}$, and $r_{\text{val},B'}^{\text{cat}}$ are 0.085, 0.039, 0.055, 0.020, 0.066, 0.043, 0.067, 0.021, 0.054 Å. Thus, the global impact of primary features on the model measured by SPEs decreases as $Z_A > r_{\text{val},B}^{\text{cat}} > r_{\text{val},A} > Z_{B'} > r_{\text{val},B'}^{\text{cat}} > r_{s,B} > Z_B > r_{s,B'}^{\text{cat}} > r_{s,A}$. The high relevance of atomic radii for the description of a_0^{SISSO} is not surprising. However, the PE sensitivity analysis shows that the most impactful radii $r_{\text{val},B}^{\text{cat}}$, $r_{\text{val},A}$, and $r_{\text{val},B'}^{\text{cat}}$ are the valence orbitals of the free atoms, and they correspond to the neutral atom for the species A and to the cations for the species B and B'. Additionally,

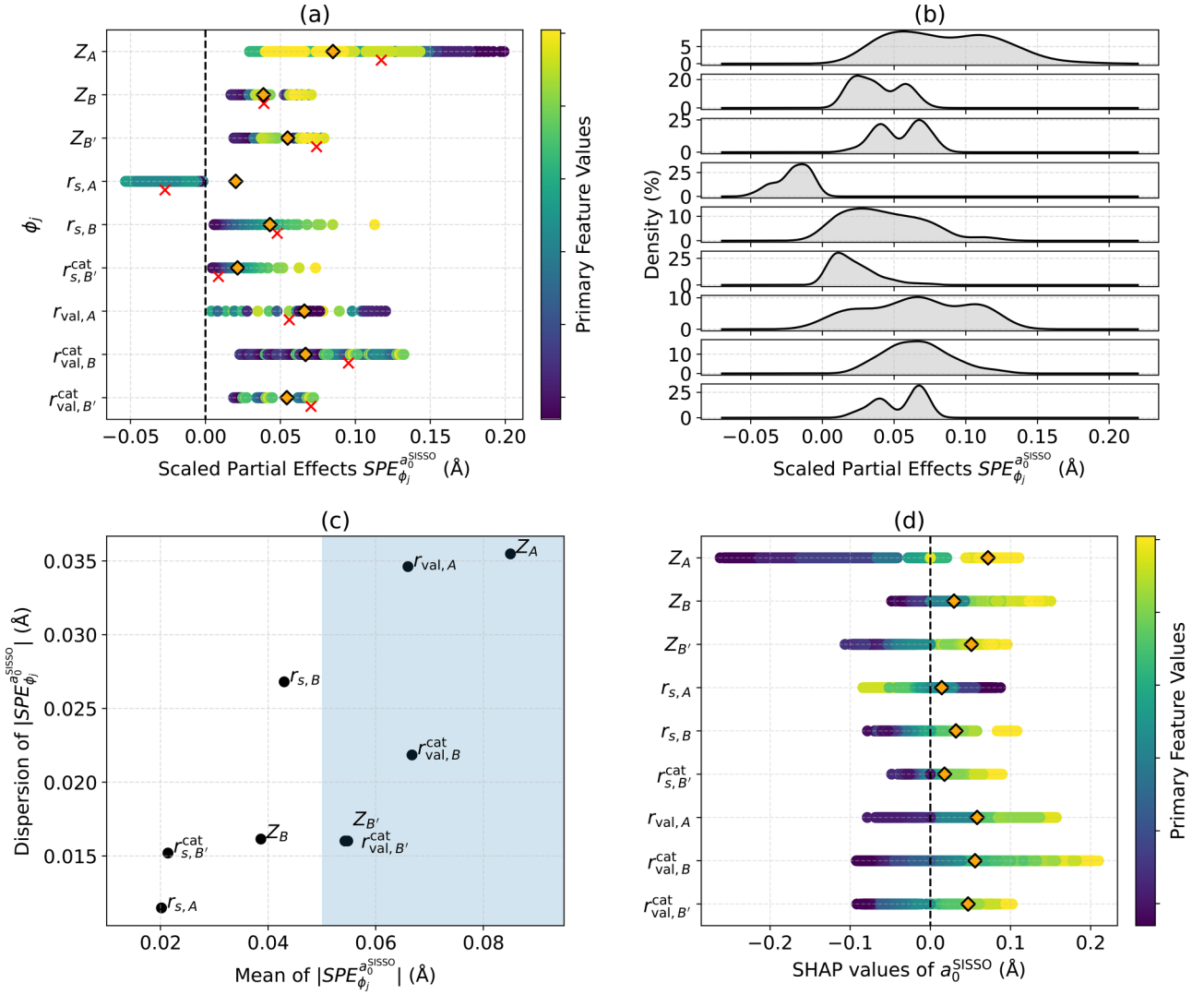


FIG. 2. (a) The scaled partial effects $SPE_{\phi_j}^{a_0^{SISSO}}$ reflect the weight of each primary feature ϕ_j on the SISSO model of the equilibrium lattice constant of cubic $A_2BB'O_6$ perovskites, a_0^{SISSO} , Eq. (1). (b) Distributions of absolute scaled partial effects $|SPE_{\phi_j}^{a_0^{SISSO}}|$. (c) Analysis of distributions of absolute scaled partial effects in terms of mean values and dispersions. (d) SHAP Analysis of the SISSO model a_0^{SISSO} . In (a) and (d), each line corresponds to one primary feature that appears in Eq. (1) and each circle represents the score for one of the 22,496 hypothetical compounds of the population. The color scales reflect the values of primary features for each material. The orange diamonds indicate the mean absolute values of the scores. The red crosses in (a) highlight the $SPE_{\phi_j}^{a_0^{SISSO}}$ values for the material Ba_2PbWO_6 .

these radii are multiplied by the respective nuclear charges (Z_A , Z_B , and $Z_{B'}$) in Eq. (1). These nuclear charges are also impactful according to the PE analysis, in particular Z_A and $Z_{B'}$. The positive signs of $SPE_{\phi_j}^{a_0^{SISSO}}$ values for most of the primary features in Fig. 2(a) indicate positive correlations of these primary features with a_0^{SISSO} . However, the $SPE_{r_{s,A}}^{a_0^{SISSO}}$ values are negative. This highlights that $r_{s,A}$ has a negative correlation with a_0^{SISSO} .

To illustrate how PEs provide local, materials-specific insights, we analyze in more detail the $SPE_{\phi_j}^{a_0^{SISSO}}$ values associated with a specific material as an example. The SPEs for Ba_2PbWO_6 are shown as black crosses in Fig. 2(a). This is the double perovskite that presents the largest a_0 in the dataset (4.32 $\text{\AA}$). The SPEs for Ba_2PbWO_6 are close to the mean values for most of the primary features. However, $SPE_{Z_{B'}}^{a_0^{SISSO}}$

and $SPE_{r_{val,B'}^{cat}}^{a_0^{SISSO}}$ are significantly higher than the mean values. This indicates that the lattice constant of Ba_2PbWO_6 is particularly sensitive to the nuclear charge of the B' element and the radius of the B' cation. This information can be used for the design of new materials. For instance, in order to modify the Ba_2PbWO_6 to obtain a material with even larger a_0 , one should replace the B' element (tungsten) with a different element presenting higher $Z_{B'}$ and $r_{val,B'}^{cat}$ rather than modifying the B (lead) and A (barium) elements. We note that for single perovskites $B = B'$ the SPEs for primary features associated with B and B' should in principle be identical. However, Eq. (1) is not fully symmetric with respect to primary features associated with B and B' [see d_2 component in Eq. (3)]. This might result in slightly different SPE values associated with primary features related to B and B' for single perovskites.

The SISSO model of Eq. (1) is linear with respect to the descriptor components d_1 , d_2 , and d_3 . However, the SR construction of expressions within the SISSO approach utilizes nonlinear unary and binary operators to create the analytical functions in the descriptor components. Thus, SISSO captures nonlinear relationships and joint effects of two or more primary features within the descriptor component functions themselves. These joint effects are referred to as *interactions* between primary features. Figure 2(a) highlights that the $\text{SPE}_{\phi_j}^{a_0^{\text{SISSO}}}$ associated with different primary features are distributed over different ranges. The distributions of $\text{SPE}_{\phi_j}^{a_0^{\text{SISSO}}}$, shown in Fig. 2(b), can be used to understand the nature of the relationship between primary features and the target property. A narrow distribution of SPE values indicates that the relationship between a primary feature and the target property is close to linear. Indeed, the partial derivative of a linear model is a constant, which results in a distribution of SPE values with zero width. Conversely, if the distribution of SPEs associated with a given primary feature is wide, (i) the relationship between the primary feature and the target is nonlinear or (ii) this primary feature affects the model in combination with other primary feature(s). In the latter case, the interaction between primary features is important to describe the target property. In Fig. 2(c), the mean values of $|\text{SPE}_{\phi_j}^{a_0^{\text{SISSO}}}|$ are plotted along with the dispersion of the $|\text{SPE}_{\phi_j}^{a_0^{\text{SISSO}}}|$ distributions. This analysis is analogous to the Morris method [35]. The standard deviation is taken here as a measure of dispersion. However, for distributions of SPE values that significantly deviate from Gaussians, the dispersion might be defined differently, e.g., using interquartile ranges.

The values associated with the primary features Z_A and $r_{\text{val},A}$ appear at the top right of Fig. 2(c), indicating that the effects of these influential primary features on a_0^{SISSO} are nonlinear or associated with primary-feature interactions. In order to determine whether a primary feature is related to the target in a nonlinear way or its effect is combined with that of a different primary feature, we evaluated the second-order partial derivatives $\frac{\partial^2 a_0^{\text{SISSO}}}{\partial \phi_i \partial \phi_j}$, where ϕ_i and ϕ_j are primary features (materials genes) appearing in the model (see details in the SM [46]). A scaling is done using the expression $\frac{\partial^2 a_0^{\text{SISSO}}}{\partial \phi_i \partial \phi_j} \times \sigma_{\phi_i} \times \sigma_{\phi_j}$, analogous to Eq. (7). These scaled second-order derivatives can be arranged in a matrix with elements $a_{ij} = \frac{\partial^2 a_0^{\text{SISSO}}}{\partial \phi_i \partial \phi_j} \times \sigma_{\phi_i} \times \sigma_{\phi_j}$. The diagonal terms of the matrix indicate how the PEs change as the primary features associated with them vary. Thus, these terms indicate nonlinearities in the PE. The off-diagonal terms indicate how the PE associated with a primary feature changes as other primary features vary. Thus, these terms capture interdependencies or interactions among primary features. The analysis of the second-order partial derivatives of Eq. (1) (see details in the SM [46]) shows that the wider dispersions of $|\text{SPE}_{Z_A}^{a_0^{\text{SISSO}}}|$ and $|\text{SPE}_{r_{\text{val},A}}^{a_0^{\text{SISSO}}}|$ are because of the interaction between these two primary features, since the off-diagonal terms of the mentioned matrix are larger than the diagonal terms for these primary features. Indeed, in Eq. (3), these two primary features appear combined with the multiplication operator as a

product. Note that the products $Z_B \times r_{\text{val},B}^{\text{cat}}$ and $Z_{B'} \times r_{\text{val},B'}^{\text{cat}}$ also appear in Eq. (1). However, the analysis in Fig. 2(c) indicates that the interactions between these primary features are not as crucial as the interaction between Z_A and $r_{\text{val},A}$. For instance, the dispersions of $|\text{SPE}_{r_{\text{val},B}}^{a_0^{\text{SISSO}}}|$ and $|\text{SPE}_{Z_A}^{a_0^{\text{SISSO}}}|$ are significantly lower than those of $|\text{SPE}_{Z_A}^{a_0^{\text{SISSO}}}|$ and $|\text{SPE}_{r_{\text{val},A}}^{a_0^{\text{SISSO}}}|$. This conclusion would have hardly been reached by the analysis of the model analytical equation. The primary features $Z_{B'}$ and $r_{\text{val},B'}^{\text{cat}}$ appear at the bottom right of Fig. 2(c), indicating that the effects of these influential primary features on a_0^{SISSO} are relatively more linear. Overall, the analysis of Fig. 2(c) reveals the most crucial nonlinearities and interactions among primary features for modeling a certain materials property target with SISSO. In the present model, this analysis highlights the importance of the product $Z_A \times r_{\text{val},A}$ for describing the target property.

We also evaluated PEs for the top 50 SISSO models, ranked according to the training RMSE (Fig. S4 within the SM [46]). As in other previous studies, we observe that different primary features are selected by SISSO compared to those selected in the best model of Eq. (1), and the SPEs change accordingly. For instance, in the second-best model {training RMSE = 0.048 Å, Eq. (S5) in the SM [46]}, SISSO selects $r_{\text{val},B'}$ instead of $r_{\text{val},B}^{\text{cat}}$. The latter primary feature has a similar SPE score in the second-best model compared to that of the former primary feature in the top-ranked model. The remaining eight primary features are the same in both models. In the third-best model {training RMSE = 0.049 Å, Eq. (S6) in the SM [46]}, SISSO selects $r_{\text{val},B}$ and $r_{\text{val},B'}$ instead of $r_{\text{val},B}^{\text{cat}}$. The SPE associated with $r_{\text{val},B}^{\text{cat}}$ in this model is reduced compared to the SPE value of this feature in the top-ranked model, whereas the SPE associated with $r_{\text{val},B'}$ is rather high. Thus, the set of primary features required to describe a given correlation by SISSO is not unique. The PE analysis identifies different and equivalent sets of key primary features that describe the target materials property with similar quality. These different sets of parameters encode the same physical information. Besides, we note that SISSO is able to reconstruct the information contained in a given primary feature by utilizing other primary features that are correlated with the given one or by combining other primary features via mathematical operators. This is a crucial aspect when modeling intricate materials properties, since not all the relevant physical parameters are typically known beforehand and some of them might be missed by the user. Of course, there is no guarantee that this always works. If important primary features are missed and such information cannot be reconstructed based on the offered primary features, the accuracy of the models identified by SISSO will be low. The good performance of an ensemble of SISSO models generated by training datasets created with primary-feature dropout [48] can also be related to such reconstruction of information.

Finally, we compare the PE approach with the SHAP [9] analysis shown in Fig. 2(d). PEs quantify the sensitivity of the model with respect to the primary features, while SHAP distributes the difference between a prediction and the mean prediction across the primary features. The global absolute SHAP scores associated with the a_0^{SISSO} model for the

primary features Z_A , Z_B , $Z_{B'}$, $r_{s,A}$, $r_{\text{val},A}$, $r_{s,B}$, $r_{\text{val},B}^{\text{cat}}$, $r_{s,B'}^{\text{cat}}$, and $r_{\text{val},B'}^{\text{cat}}$ are 0.073, 0.030, 0.052, 0.015, 0.033, 0.019, 0.059, 0.056, 0.048 Å. Thus, the global impact of primary features measured by SHAP is $Z_A > r_{\text{val},B}^{\text{cat}} > r_{s,B'}^{\text{cat}} > Z_{B'} > r_{\text{val},B'}^{\text{cat}} > r_{\text{val},A} > Z_B > r_{s,B} > r_{s,A}$. This ranking is similar to that obtained by SPEs in Fig. 2(a), with the exception of the primary features $r_{\text{val},A}$ and $r_{\text{val},B}^{\text{cat}}$, which are ranked in the inverse order. Overall, the PE analysis recovers the insights obtained with SHAP. This result is consistent with previous works showing that PEs reflect the ranking provided by Shapley values [41,42]. Additionally, PEs provide a more intuitive interpretation on the impact of the primary features, since positive or negative values reflect direct and inverse correlations. Finally, we note that the PE approach is more computationally efficient than SHAP, and it circumvents the assumptions and approximations utilized in the SHAP analysis (see details in the SM [46]). Indeed, the evaluation of PEs does not require the generation of new input samples in which the values of primary features are modified, since the partial derivatives are evaluated for the actual materials of the dataset. This is an advantage with respect to SHAP and other widely used sensitivity methods, which require knowledge or assumptions about correlations between primary features in order to ensure that only physically meaningful input samples that correspond to real materials are generated [11,39,49].

III. CONCLUSIONS

Overall, the PE sensitivity analysis applied to a SISSO study enables an efficient identification of the core, most

relevant primary features to describe materials properties (“materials genes”) via analytical derivatives. The example used in the discussion above concerned the SISSO description of the equilibrium lattice constant of cubic perovskites. In the same spirit, the PE sensitivity analysis has also been applied to heterogeneous catalysis [30]. The PE analysis also reveals how distinct gene combinations encode equivalent information. The PEs identify the radii of valence orbitals of free atoms of elements A , B , and B' and atomic numbers (Z) as the most influential physical parameters for describing the equilibrium lattice constant of $A_2BB'O_6$ perovskites, out of 23 offered physical parameters. While it is not surprising that the lattice constant is described by the mentioned radii, the sensitivity analysis showed that nontrivial interactions between radii and atomic numbers, in particular the product $Z_A \times r_{\text{val},A}$, are key to modeling the target property. Therefore, the sensitivity analysis improves the interpretability of SISSO models and enables materials-specific physical insights.

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DATA AVAILABILITY

The dataset and a Jupyter notebook allowing to reproduce the AI analysis are available at [56].

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