

Giant spontaneous polarization in zinc-blende III-V semiconductorsJ. Cañas^{1,2,*}, M. Yassine^{1,†}, and O. Ambacher¹¹*Power Electronics, Institute for Sustainable Systems Engineering INATECH, University of Freiburg, Emmy-Noether-Str. 2, D-79110 Freiburg, Germany*²*Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France*

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The discovery of ferroelectricity in wurtzite nitrides has paved the way for measuring and understanding spontaneous polarization in III-V semiconductors. However, the calculation of polarization effects at heterointerfaces, crucial for numerous electronic and photonic applications, remains a topic of debate. The need for a reference structure to calculate spontaneous polarization has led to discussions over whether to use the zinc-blende or layered hexagonal structures as the reference for wurtzite crystals. In this Letter, we argue that the layered hexagonal structure is not only a better reference due to its vanishing formal polarization, but also the appropriate choice for the wurtzite system to reproduce the polarization values observed in ferroelectric switching experiments. This leads to the idea of using ferroelectricity as a basis for defining spontaneous polarization. Applying this definition, we extend our analysis to III-V zinc-blende semiconductors and reveal that they can exhibit a spontaneous polarization approximately three times larger than that of wurtzite, thereby refuting the longstanding assumption that it is zero. Through this example, we illustrate that spontaneous polarization is not inherently linked to charge density at interfaces.

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The recent measurement of ferroelectricity in wurtzite ScAlN has established a basis for understanding spontaneous polarization in III-V semiconductors [1]. The need for a reference structure to calculate spontaneous polarization has led to a debate over whether to use the zinc-blende [2] or layered hexagonal [3] structures as the reference for wurtzite crystals. Due to this discrepancy, the polarization effects at heterointerfaces—critical for key applications such as light-emitting diodes (LEDs) and high-electron-mobility transistors (HEMTs)—remain a subject of discussion. The choice of reference significantly impacts the deduced values of spontaneous polarization, differing by orders of magnitude. However, predicted values for polarization-bound charges at conventional nitride interfaces show only slight variations. Notably, when stacking different crystal types, giant polarization discontinuities have been predicted using the layered hexagonal reference [4,5]. This striking yet experimentally unverified prediction [6] has led much of the nitride research community to rely on spontaneous polarization values derived from the zinc-blende reference.

In this Letter, we address this discrepancy by revisiting the definition of spontaneous polarization, grounding it in the context of ferroelectric switching, which connects it to a

physically measurable polarization difference [7,8]. Indeed, the measured values of spontaneous polarization from ferroelectric measurements in wurtzite nitrides align with calculations that use the layered hexagonal structure as a reference. This is because the layered hexagonal structure represents an intermediate centrosymmetric phase between the polarities of wurtzite [9]. Moreover, we extend this definition to study the III-V zinc-blende semiconductor system. We show that zinc-blende semiconductors can exhibit giant spontaneous polarization up to three times that of wurtzite crystals, contrary to the historical belief that it has no spontaneous polarization. Through this example, we demonstrate that spontaneous polarization is not necessarily related to polarization-bound charges at interfaces.

Under the modern theory of polarization, the formal polarization (P_f) of a crystal is determined as the sum of two components: ionic polarization, which arises from the contribution of atomic nuclei and is computed using the classical description of dipoles, and electronic polarization, which originates from the valence electrons and is calculated using the Berry phase approach [8,10,11]:

$$P_f = \frac{e}{\Omega} \sum_s Z_s^{\text{ion}} R_s^{(\lambda)} + \frac{ie\Omega}{(2\pi)^3} \sum_j^{\text{occ.}} \int_{\text{BZ}} dk \langle u_{j,k}^{(\lambda)} | \Delta_k | u_{j,k}^{(\lambda)} \rangle. \quad (1)$$

The first term is the ionic contribution (P_{ion}), calculated as the sum of the product of the ionic charges Z_s and the nuclei positions R_s over the unit cell volume Ω . The second term is the electronic contribution (P_{el}), calculated through the Berry potential $\langle u_{j,k}^{(\lambda)} | \Delta_k | u_{j,k}^{(\lambda)} \rangle$ of the cell-periodic crystal Bloch wave functions $|u_{j,k}^{(\lambda)}\rangle$ integrated over the Brillouin zone.

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This second term represents the electronic polarization as the sum of the product of the electronic charge and the Wannier centers.

The formal polarization corresponds to the dipolar moment of a primitive unit cell divided by its volume. As a result, the formal polarization depends on the location (and the shape) of the primitive unit cell. As there are multiple choices of primitive cell to describe a crystal, the polarization of an infinite crystal becomes a multivalued quantity forming a polarization lattice rather than a single value, as explained by Spaldin [12]. This multivalued nature emerges directly from the crystal's periodicity and the invariance under unit cell translation [8,12,13]. The multivalued character of polarization gives rise to the polarization quantum (P_q), which separates the different values (branches) of polarization. P_q is given by eR/Ω , where R is the vector along which the polarization is calculated. Consequently, the polarization of a crystal is not uniquely defined, and only differences in formal polarization (within the correct polarization branch) have physical significance. Indeed, this is also the case for experimental measurements of polarization, as all polarization-induced effects (such as interface charges, ferroelectric switching, or piezoelectric effect) are always observed through polarization differences.

The definition of spontaneous polarization has been a longstanding challenge within the nitride community. Bernardini *et al.* proposed defining the spontaneous polarization of wurtzite by taking its formal polarization difference with a zinc-blende reference [2]. The intuition behind this approach is that the spontaneous polarization of zinc-blende is zero, and both wurtzite and zinc-blende structures are tetrahedrally coordinated. Therefore, any structural deviations from the ideal wurtzite structure would lead to a formal polarization difference relative to its zinc-blende counterpart, giving rise to spontaneous polarization. While the definition of such a formal polarization difference is theoretically sound, referring to it as spontaneous polarization is somewhat arbitrary, as other reference structures could be chosen ambiguously. Moreover, there is no straightforward transformation from a wurtzite to a zinc-blende structure [2,8,12]. The lack of ferroelectricity in these materials until recent discoveries [1] created a disconnect between the nitride and ferroelectric research communities. While the ferroelectric community had established a clear understanding of spontaneous polarization [8], this separation allowed an unconventional definition of spontaneous polarization to persist within the nitride community for many years [2].

Therefore, as in the work by Dreyer *et al.* [3], the most logical reference for wurtzite is a layered hexagonal structure, which is centrosymmetric, nonpolar, and has vanishing formal polarization (modulo P_q). At first glance, this choice may seem just convenient but unconventional, as there is no experimental evidence of such a structure for InN, GaN, or AlN. However, the layered hexagonal structure serves an intermediate point in the fictitious ferroelectric switching path for wurtzite, directly linking it to experimental ferroelectric measurements of polarization [9]. This approach allows spontaneous polarization to be defined as the ferroelectric switching polarization: either as the formal polarization difference between the wurtzite and layered hexagonal structures, or as half the formal polarization difference between the two

wurtzite polarities along the switching path through the layered hexagonal structure.

A few conceptual clarifications are necessary at this point. The formal polarization lattice is the fundamental quantity defined by the crystal's symmetry and electronic structure. Spontaneous polarization, on the other hand, corresponds to the idea of physical manifestation of polarization. However, since only differences in formal polarization have a physical meaning, the spontaneous polarization of a polar structure always has to be defined relative to another structure. Even when defined through ferroelectric switching, by comparing two oppositely polarized states of the same material, the specific switching path determines the value of the spontaneous polarization (through quantum polarization integers), not solely the endpoint structures.

It is therefore important to note that any formal polarization difference used to define a physical manifestation of polarization is valid, provided an insulating interface can be constructed between the two materials [14]. Bernardini *et al.*'s definition of spontaneous polarization represents the physical manifestation of a polarization gradient across a homointerface between lattice-matched zinc-blende and wurtzite [2]. In contrast, the definition provided by Dreyer *et al.* corresponds to the polarization change occurring during a ferroelectric switching process in wurtzite, following a path through the layered hexagonal structure [3].

However, due to the arbitrariness in the definition provided by Bernardini *et al.* [2], which compares two structures that cannot be easily connected through a continuous transformation, we seek a more consistent definition of spontaneous polarization that maintains a direct connection to the original crystal. To this end, we propose defining spontaneous polarization, using the fictitious path framework [15], as half the difference in formal polarization between the two opposite polarities of a polar structure connected by a continuous path that passes through a centrosymmetric reference structure [8,11].

This definition of spontaneous polarization is advantageous: First, it is directly linked to experimental polarization measurements through ferroelectric switching and can be validated through experiments provided that the ferroelectric switch happens in a homogeneous fashion. Second, this definition is only dependent on the original crystal and its switching path, and the choice of reference is not arbitrary—it is always a centrosymmetric, nonpolar structure that serves as the midpoint between the switching of polarities. It is also consistent with the etymological origin of the concept of spontaneous polarization within ferroelectric materials [7,8]. Note that because the layered hexagonal formal polarization is zero (modulo P_q), the value of the formal polarization of wurtzite is the same as the spontaneous polarization. Therefore, for wurtzite, *spontaneous polarization coincides with the formal polarization of a material at zero strain* [9,16].

As discussed earlier, the spontaneous polarization of a zinc-blende crystal has always been considered zero, based on the argument that its four polar triad axes cancel out any net spontaneous polarization [17]. However, the $\langle 111 \rangle$ direction of zinc-blende is polar, has a nonzero formal polarization [3], and also exhibits piezoelectricity [18]. This system is of extreme technological importance, and there are abundant experimental data for its interfaces; however, there is no

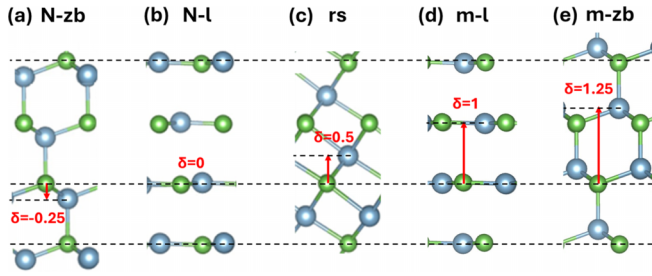


FIG. 1. Scheme of the zinc-blende N-polar to m-polar transformation along the $\langle 111 \rangle$ direction showing the ratio of the separation between planes of anions (green) and cations (blue) to the separation between planes of cations in each structure (δ). (a) Nitrogen-polar zinc-blende, (b) nitrogen-polar layered, (c) rocksalt, (d) metal-polar layered, and (e) metal-polar zinc-blende.

experimental report of ferroelectric switching of zinc-blende. To understand the spontaneous polarization of zinc-blende crystals, we can devise a transformation, analogous to the wurtzite system, that switches polarities through a centrosymmetric, nonpolar structure. This transformation is illustrated in Fig. 1, exemplified for the III-N material system. The N-polar zinc-blende is transformed by displacing metal atoms in the $\langle 111 \rangle$ direction, resulting in an N-polar layered structure (distinct from a layered hexagonal structure), and then further transforming into rocksalt, its centrosymmetric counterpart. The transformation then continues through a m-polar layered phase before reaching m-polar zinc-blende. Note that we adopt the conventional wurtzite nitride terminology to refer to N-polar zinc-blende, which, in the zinc-blende community, is commonly described as $(\bar{1}\bar{1}\bar{1})$ -oriented zinc-blende with a $(111)B$ surface or a nitrogen-terminated (111) surface [19]. This surface is stable only when terminated with nitrogen. However, polarity and surface termination are distinct concepts, even though, in practice, N-polar zinc-blende exhibits a nitrogen-terminated surface. The illustrated transformation is an extension of the one in this work by Adamski *et al.* [4] to connect rocksalt and zinc-blende. Through this transformation, which represents a fictitious ferroelectric switching path for zinc-blende, we can define its spontaneous polarization as half the formal polarization difference between its two polar states.

This system, however, exhibits more subtleties than its wurtzite counterpart. Notably, the formal polarization of its centrosymmetric structure (rocksalt) is nonzero. It is impossible to construct a stoichiometric rocksalt primitive unit cell that has no dipole along the $\langle 111 \rangle$ direction; in fact, the minimum absolute value of formal polarization is $P_q/2$ [4,20]. However, in finite crystals, such large polarizations are not observed experimentally, as they are mitigated by external species, incomplete surface coverage, or rough, non-polar surface reconstructions [21,22]. Consequently, in the case of zinc-blende, when the spontaneous polarization is defined through a ferroelectric switching path that passes through the rocksalt structure, the resulting value does not appear in the formal polarization lattice, unlike in the wurtzite system.

We have calculated the formal polarization along the zinc-blende N-polar to m-polar transformation shown in Fig. 1 using the PWSCF code of the QUANTUM ESPRESSO (QE) software package [23,24]. The unit cell consisted of six atoms for all the materials considered. We used the generalized gradient approximation Perdew-Burke-Ernzerhof (PBE) functional for exchange correlation. The wave functions of the valence electrons are represented by a plane-wave basis set with a cutoff energy of 70 Ry and the electron density and effective Kohn-Sham potential by discrete Fourier series with a cutoff energy of 560 Ry. The interactions of valence electrons with the atomic nuclei and core electrons are described by pseudopotentials taken from the open-source Standard Solid State Pseudopotentials (SSSP PBE Efficiency v1.3.0) library [25]. Brillouin zone integrals were evaluated on a Monkhorst-Pack mesh of $15 \times 15 \times 30$ k points. The convergence threshold was set to 10^{-8} Ry for the total energy and to 10^{-6} Ry/Bohr for the forces on atoms. We have verified that the crystals preserved a band gap throughout the transformation.

In Fig. 2, we show the formal polarization calculated for the structures under the ferroelectric switch of zinc-blende for GaAs and AlAs in Fig. 2(a) and GaN and AlN in Fig. 2(b) in the branch showing $P_f^s = 0.5P_q$. The δ parameter is defined as the ratio of the separation between planes of anions and cations to the separation between planes of cations [4]. The spontaneous polarization, deduced as half the formal polarization difference between the two zinc-blende polarities, is smaller for arsenides ($P_{sp}^{\text{GaAs}} = 2.521$ C/m² and $P_{sp}^{\text{AlAs}} = 2.534$ C/m²) than for nitrides ($P_{sp}^{\text{GaN}} = 4.024$ C/m² and $P_{sp}^{\text{AlN}} = 4.293$ C/m²) due to their larger unit cells.

The consistent definition of spontaneous polarization enables us to demonstrate that, contrary to historical belief, zinc-blende does indeed have a nonzero spontaneous polarization, in addition to its well-known nonzero formal polarization [3]. Remarkably, the spontaneous polarization of zinc-blende, defined through the ferroelectric switching path via the rocksalt phase, is about three times larger than its wurtzite counterpart for each of the materials.

Additionally, this system provides an interesting example of the fundamental difference between spontaneous polarization, defined through ferroelectric switching, and formal polarization. While spontaneous polarization is strictly related to ferroelectric properties and depends on the switching path, formal polarization can be used to predict charge gradients between epitaxially grown crystals, as described in the interface theorem by Vanderbilt *et al.* [14]. In the case of a zinc-blende/rocksalt interface, the large difference in formal polarization is expected to give rise to a significant interface charge density, in the fashion of the theoretically predicted polarization gradient between wurtzite and rocksalt [4]. However, the difference in spontaneous polarization, defined via the respective fictitious ferroelectric switching paths for wurtzite and for zinc-blende, has no direct physical meaning; that is, it cannot be used to predict correct interfacial charge densities.

Interestingly, the formal polarization of zinc-blende always takes the same value in III-V materials, expressed in quantum

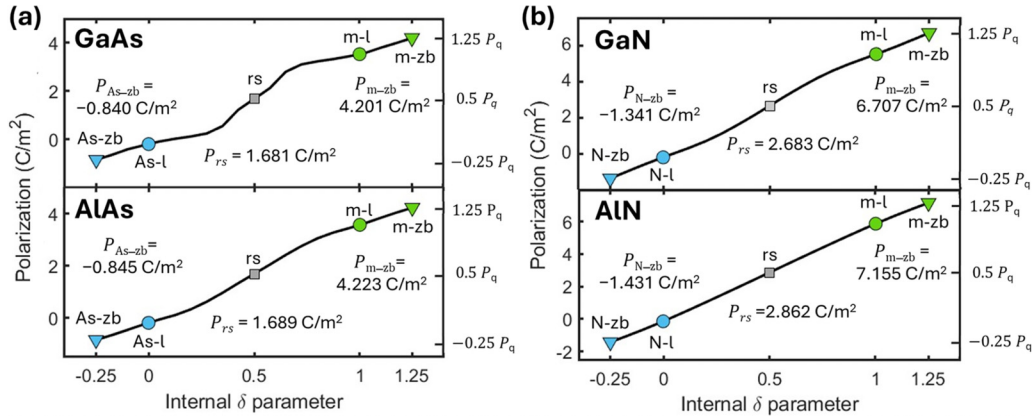


FIG. 2. Formal polarization calculated for the structures under the zinc-blende N-polar to m-polar transformation for (a) GaAs and AlAs and for (b) GaN and AlN for a branch with $P_f^{rs} = 0.5P_q$.

of polarization units (P_q), as it does for rocksalt ($P_f^{rs} = 0.5P_q$). For zinc-blende, the formal polarization is always $-0.25P_q$ for the group-V polar structure and $1.25P_q$ for the group-III polar structure. This implies that the formal polarizations of zinc-blende (and rocksalt) do not explicitly depend on the atoms involved in bonding, but only on the volume of the unit cell (Ω) via P_q . More precisely, the quantum of polarization for this transformation depends only on the basal plane area (A_b) of the unit cell: $P_q = e/A_b$. The ionic contribution to the formal polarization will always be the same, as the valence of the elements is the same for III-V materials, and only the ionic contribution from electrons involved in bonding is considered (the rest of the nucleus charge is screened). While the wave functions describing the electronic bonding between different nitrides and arsenides are indeed different, the symmetry of the zinc-blende and rocksalt lattices ensures that the electronic part of the polarization always cancels out. As for rocksalt, no large surface charge is observed (111)-oriented freestanding zinc-blende crystals, due to its non vanishing formal polarization, as a result of its passivation with external species or partial coverage [26,27].

There is no experimental evidence of ferroelectric switching in zinc-blende structures. However, piezoelectric and pyroelectric-like effects have been observed experimentally [28] resulting from changes in the δ parameter. This means that when the zinc-blende structure is uniaxially deformed in the $\langle 111 \rangle$ direction, the cation-to-anion distance changes, deviating from that in the ideal zinc-blende structure. This leads to a nonzero contribution from the electronic part of the polarization, resulting in piezoelectricity and a formal polarization $P_f \neq 0.25P_q$. In fact, this occurs whenever a zinc-blende A layer is epitaxially grown on top of another zinc-blende B. The A layer adopts the in-plane lattice parameter of B and deforms in the $\langle 111 \rangle$ direction, modifying its δ . The formal polarization of the B layer is $P_f^b = 0.25P_q^b$, while the epitaxial A layer has a formal polarization $P_f^a = (0.25 + \alpha)P_q^b$, where α is the change of the formal polarization due to the nonideal δ parameter. While in the case of GaAs/AlAs interfaces, the lattice mismatch is small enough that this effect (α) is negligible, interface charges between lattice-mismatched zinc-blende structures are well explained by this phenomenon [18].

The reason ferroelectric switching has never been observed experimentally in zinc-blende is due to the large energy barrier for switching and the associated high coercive electric field. In Fig. 3, we show the energies per atom calculated for the structures under the ferroelectric switch of zinc-blende for GaAs and AlAs in Fig. 3(a) and GaN and AlN in Fig. 3(b). The curves for the arsenides show two local maxima at similar energies, one near the layered structure and the other for rocksalt. AlN also displays its maximum energy configuration near the layered structure, but rocksalt is a local minimum. For GaN, the maximum energy is located at rocksalt, significantly higher than that for the layered structures. Specifically, for arsenides and aluminum nitride, the energy barrier is about 0.5 eV/atom, while for GaN, it exceeds 0.6 eV/atom. These barriers are roughly double the energy required to switch conventional binary nitrides wurtzite structures, which already requires very large coercive fields. For instance, coercive fields are experimentally over the critical electric field (~ 10 MV/cm) for wurtzite AlN. This is why its ferroelectric properties were not experimentally observed until recently, when alloying it with ScN helped lower the coercive field [1]. Indeed, the estimated coercive fields for the studied zinc-blende materials, based on our calculations, should exceed 40 MV/cm, making the switching of binary nitrides or arsenides impossible, as their critical fields are much lower. Furthermore, while the zinc-blende phase has a band gap close to that of wurtzite, the rocksalt phase has a smaller band gap and thus a smaller critical electric field, making it even more difficult to sustain the coercive field without breakdown. As shown, even if the transformation exists, its switching barrier is too high for the material to sustain the transformation. However, as with wurtzite, group-III transition metal ternary alloys can lower the rocksalt energy [29]. It is intriguing whether it is possible to find a material candidate with a low enough coercive field for switching zinc-blende. However, it remains unclear whether alloys with such transition metals would lower the energy for the layered structures, as they may still present the maximum energy barrier for the ferroelectric switching of zinc-blende. Nonetheless, the definition of spontaneous polarization in this phase is unambiguous and rigorous. Even though the ferroelectric switch of this phase is hardly achievable experimentally, the spontaneous polarization

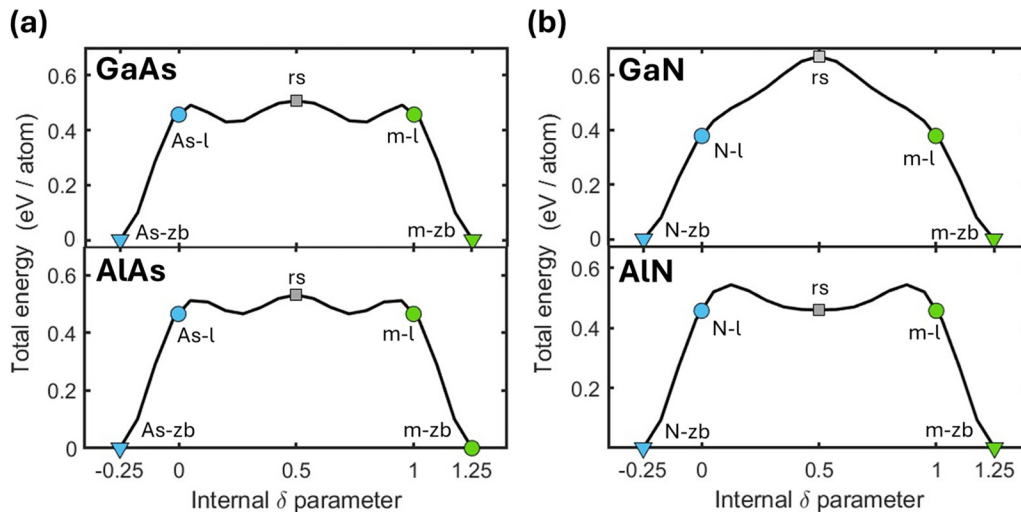


FIG. 3. Energy per atom calculated for the structures under the zinc-blende N-polar to m-polar transformation for (a) GaAs and AlAs and (b) GaN and AlN.

value is well defined as half the formal polarization difference between its polar phases through the rocksalt path. Alternatively, a potential strategy to demonstrate ferroelectric switching in zinc-blende could involve inducing it through proximity switching of a ferroelectric wurtzite nitride [30].

In conclusion, we have examined the definition of spontaneous polarization and highlighted the advantages of adopting a more consistent framework based on ferroelectric switching. This approach provides a nonarbitrary, nonpolar, centrosymmetric reference structure connected to the polar crystal via a fictitious ferroelectric switching path. Extending this definition to the zinc-blende case, we identified a transformation along the (111) direction, switching zinc-blende N-polar to m-polar through the nonpolar centrosymmetric rocksalt structure. Using this transformation, we have shown that the spontaneous polarization associated with the ferroelectric switch of zinc-blende is about three times higher than that

of wurtzite, contrary to the historical belief that it is zero. We have explained how this fact is compatible with the experimental observations of piezoelectricity, interface bound charges, and the absence of polarization effects in freestanding crystals of zinc-blende. The ferroelectric coercive field of zinc-blende materials is too large compared to their typical critical electric fields, preventing ferroelectric switching in the studied materials, which explains the absence of experimental evidence.

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J.C. and M.Y. contributed equally to this work.

The data that support the findings of this article are openly available [31].

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