



**CHALMERS**  
UNIVERSITY OF TECHNOLOGY

## **Massive Discovery of Low-Dimensional Materials from Universal Computational Strategy**

Downloaded from: <https://research.chalmers.se>, 2026-04-15 09:44 UTC

Citation for the original published paper (version of record):

Bagheri, M., Berger, E., Komsa, H. et al (2026). Massive Discovery of Low-Dimensional Materials from Universal Computational Strategy. *Chemistry of Materials*, 38(5): 2395-2402.  
<http://dx.doi.org/10.1021/acs.chemmater.5c03151>

N.B. When citing this work, cite the original published paper.

# Massive Discovery of Low-Dimensional Materials from Universal Computational Strategy

Mohammad Bagheri,\* Ethan Berger, Hannu-Pekka Komsa, and Pekka Koskinen\*



Cite This: *Chem. Mater.* 2026, 38, 2395–2402



Read Online

ACCESS |



Metrics & More

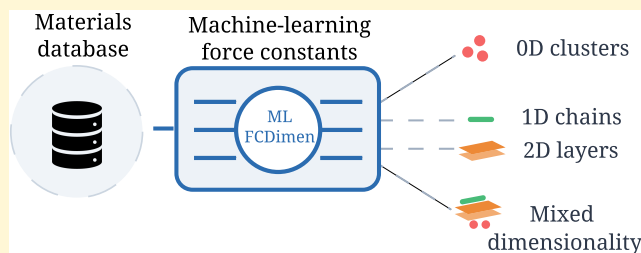


Article Recommendations



Supporting Information

**ABSTRACT:** Low-dimensional materials have attractive properties that drive intense efforts toward the discovery of novel materials. However, experiments are tedious for systematic discovery, and the present computational methods are often tuned to two-dimensional (2D) materials, overlooking other low-dimensional materials. Here, we combined universal machine-learning interatomic potentials (UMLIPs) and an advanced, interatomic force constant (FC)-based dimensionality classification method to make a massive discovery of novel low-dimensional materials. We first benchmarked the UMLIPs' first-principles-level accuracy in quantifying FCs and calculated phonons for 35,689 materials from the Materials Project database. We then used the FC-based method for dimensionality classification to discover 9139 low-dimensional materials, including 1838 0D clusters, 1760 1D chains, 3057 2D sheets/layers, and 2484 mixed-dimensional materials, all of which conventional geometric descriptors have not recognized. By calculating the binding energies for the discovered 2D materials, we also identified 887 sheets that could be easily or potentially exfoliated from their parent bulk structures.



## INTRODUCTION

The discovery of novel functional materials for targeted applications has long been central to materials research. Over the past two decades, the rise of graphene has revealed remarkable properties that have sparked a quest for novel two-dimensional (2D) materials with ever-growing attention.<sup>1</sup> To date, the quest has unearthed numerous 2D materials such as transition-metal dichalcogenides (TMDs), MXenes, metal-LENES, and emerging non-van der Waals systems, offering promising applications in electronics,<sup>2–6</sup> optics,<sup>7–9</sup> magnetism,<sup>10–12</sup> sensors,<sup>13–15</sup> catalysis,<sup>16–19</sup> and topological materials.<sup>20–23</sup>

Another approach to materials discovery is computation. Many studies have employed high-throughput computations and data-driven approaches to systematically screen thousands of experimentally known bulk materials, uncovering hundreds to over a thousand exfoliable 2D material candidates.<sup>24–31</sup> Yet these efforts have been targeted at 2D materials, with only scant studies systematically addressing materials with zero-dimensional (0D), one-dimensional (1D), or mixed-dimensional characteristics.<sup>32–35</sup>

To identify materials' low-dimensional character, most computational methods use geometrical criteria, such as atomic positions and atomic radii.<sup>36–39</sup> This approach has often proven to be reasonable for dimensionality identification. Geometries are usually calculated by density-functional theory (DFT), which is the workhorse method that is accurate enough for predicting materials and their properties. Yet even a realistic geometry can be inaccurate for dimensionality

prediction because it relies on empirical correlations between the lengths and strengths of atomic bonds. This shortcoming was recently remedied by a method that uses interatomic force constants (FCs) to identify low-dimensional units from bulk materials.<sup>40</sup> While this method—FCDimen—has the merit of relying on chemical bonding quantitatively, so far its applicability has been limited by the high cost of DFT-level calculation of FCs.

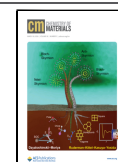
Fortunately, universal machine-learning interatomic potentials (UMLIPs) have recently become increasingly helpful in reducing calculation time and generating results at DFT-level accuracy.<sup>41–43</sup> UMLIPs are trained by massive datasets and aim for applicability to all materials that contain nearly all elements. Although trained to predict only energies and forces, UMLIPs have been shown to reliably predict their derivatives as well, such as formation energies of bulk materials,<sup>44</sup> defect formation energies,<sup>45</sup> and phonon dispersion curves.<sup>46</sup> It would be reasonable to expect that UMLIPs would also be applicable in predicting FCs for the fast and reliable identification of low-dimensional units.

Received: November 21, 2025

Revised: February 13, 2026

Accepted: February 19, 2026

Published: February 24, 2026



Therefore, in this article, we used UMLIPs to calculate FCs and FCDimen to determine the dimensionalities of 35,689 materials from the Materials Project (MP) database.<sup>47</sup> To choose the most accurate model, we benchmarked two UMLIPs, MatterSim<sup>48</sup> and MACE,<sup>49,50</sup> against DFT-calculated phonon properties and FCs of an existing phonon database with more than 10K materials.<sup>46,51</sup> We then compared the FCDimen-predicted dimensionalities that DFT and UMLIPs gave for these materials and concluded that MatterSim is sufficiently accurate for predicting material dimensionalities. Leveraging on MatterSim, we screened 153,234 bulk materials and discovered 9139 low-dimensional materials, including 2D sheets, 1D chains, 0D clusters, and various mixed dimensionalities. Finally, by calculating the interlayer binding energies for the discovered 2D sheets, we found that 887 of them—all new to the known 2D materials databases—are easily or potentially exfoliable from their parent bulk structure.

## METHODS

### Computational Methods

The machine-learning (ML) calculations were performed using MatterSim with the pretrained model v1.0.0–5M<sup>48</sup> and MACE<sup>49,50</sup> with the pretrained large model of MACE-MP-0 (MACE-MP-0b3) without dispersion corrections. The MatterSim-v1 model is based on the M3GNet<sup>52</sup> architecture, which was trained on relaxations obtained from the Materials Project.<sup>47</sup> Both UMLIP models are available as calculators in the Atomic Simulation Environment (ASE).<sup>53</sup> ASE was used, with the help of Python, to construct the calculation workflow. In the benchmark, all parameters were kept the same as those in the Phonon database.<sup>51</sup> All materials were relaxed using the FIRE<sup>54</sup> and BFGS algorithms to forces below 1 meV/Å. The crystal structures and their properties were extracted using MP-API<sup>55</sup> and Python materials genomics (pymatgen).<sup>56</sup> The space groups were calculated using spglib<sup>57</sup> with a symmetry precision of 10<sup>−6</sup>.

Initial dimensionalities were calculated using Larsen's<sup>37</sup> method, which is implemented in ASE.<sup>53</sup> Phonon calculations were done using the Phonopy package,<sup>58,59</sup> using a displacement of 0.01 Å. The supercell sizes used for determining the force constants were chosen so that the number of atoms was less than or equal to 250 while keeping the point groups of the Bravais lattices of the conventional unit cell and the supercell the same.

Initial structures of known 2D materials (Figure 4a) were extracted from ref 27. All density-functional theory calculations were performed using VASP (Vienna Ab initio Simulation Package) software,<sup>60,61</sup> together with the projector-augmented wave method.<sup>62</sup> The Becke–Johnson (BJ) damping variant of the DFT-D3 functional was adopted.<sup>63</sup> The plane wave cutoff was set to 520 eV. The Brillouin zone of the unit cell was sampled by a  $\Gamma$ -centered  $k$ -point mesh whose density was defined by  $R_k = 20$ , which in VASP determines the subdivisions  $N_1$ ,  $N_2$ , and  $N_3$  along the reciprocal lattice vectors  $b_1$ ,  $b_2$ , and  $b_3$ , respectively, via  $N_i = \max(1, R_k|b_i| + 0.5)$  and rounded to an integer. The energy convergence criterion between consecutive steps was set to 10<sup>−8</sup> eV for the self-consistent loop and 10<sup>−6</sup> eV for ionic relaxation. Structures were considered to be relaxed when no force exceeded 1 meV/Å.

In the machine-learning binding energy calculation, we employed torch-dftd3<sup>63–66</sup> alongside MatterSim to add the D3 correction in our calculations to correct the weak van der Waals (vdW) interaction. This approach has already proven successful for the investigation of 2D material heterobilayers.<sup>67</sup>

### Binding Energy Calculation

The method used to obtain the binding energy  $E_b$  is adapted from ref 24. Taking materials from the MP, the bulk unit cell is first relaxed with a D3 correction to obtain the initial energy  $E_0$  as well as the force constant. Using the latter, 2D units are identified using FCDimen.

The resulting monolayers are then isolated and relaxed, leading to the layer energies  $E_l$ . The binding energy  $E_b$  is then found as

$$E_b = \frac{\sum E_l - E_0}{A \cdot N_l} \quad (1)$$

where  $N_l$  is the number of layers in the unit cell and  $A$  is the area of the layers.

## RESULTS

### FCDimen

We begin by briefly reviewing the FC-based dimensionality classification approach FCDimen previously introduced in ref 40. For a system with potential energy  $U(\mathbf{r}_1, \dots, \mathbf{r}_n)$ , where  $n$  is the number of atoms and  $\mathbf{r}_i$  is the position of atom  $i$ , the force on atom  $i$  is

$$F_i^\alpha = -\frac{\partial U}{\partial \mathbf{r}_i^\alpha} \quad (2)$$

where  $\alpha$  is the Cartesian coordinate index. The FC between the coordinates  $\alpha$  and  $\beta$  of atoms  $i$  and  $j$  is

$$\Phi_{ij}^{\alpha\beta} = \frac{\partial^2 U}{\partial \mathbf{r}_i^\alpha \partial \mathbf{r}_j^\beta} = -\frac{\partial F_i^\alpha}{\partial \mathbf{r}_j^\beta} \quad (3)$$

A scalar magnitude of the FC between atom pair  $ij$  is given by reducing the  $3 \times 3$  tensor using the Frobenius norm

$$\Phi_{ij} = \left\| \Phi_{ij}^{\alpha\beta} \right\|_F \quad (4)$$

The strongest bond for atom  $i$  can be identified by defining the maximum FC for each atom as

$$\Phi_i^{\max} = \max_{j \neq i} (\Phi_{ij}) \quad (5)$$

which allows us to quantify the minimum and maximum bond strengths in the material as

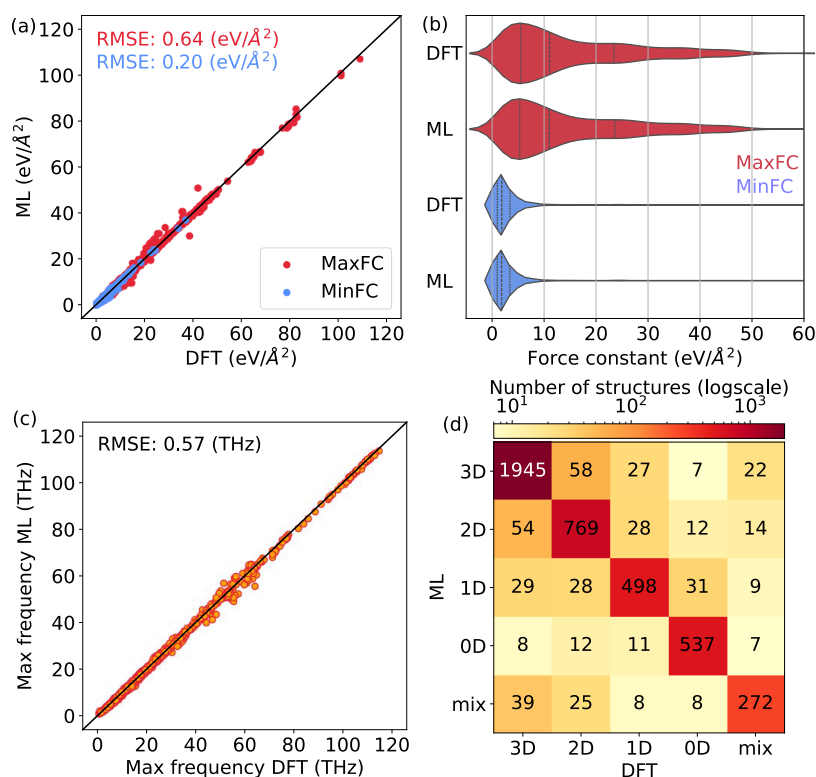
$$\text{MinFC} = \min_i (\Phi_i^{\max}), \text{ and}$$

$$\text{MaxFC} = \max_i (\Phi_i^{\max}). \quad (6)$$

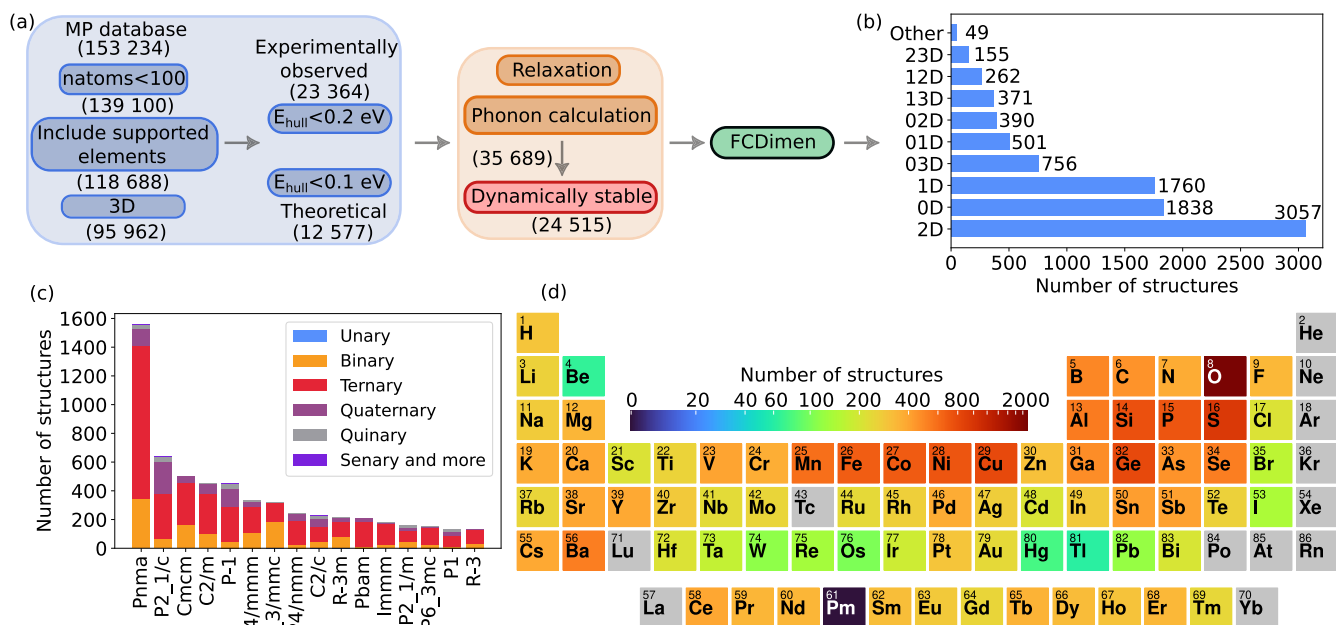
To identify low-dimensional units, we treat the atoms as nodes in a graph. A pair of atoms is considered connected when the interatomic FCs are larger than a threshold  $t = \text{MinFC}$ , i.e., when  $\Phi_{ij} \geq t$ . The low-dimensional units are then defined as the resulting connected components of atoms linked by bonds. The dimensionality of these components is determined by the periodic extension of their unit cell (e.g., a component connected to its own periodic image in two directions is classified as 2D). Furthermore, scanning the threshold between  $t = \text{MinFC} \dots \text{MaxFC}$  gives a score in the range 0–1 for the assigned dimensionality. The FCDimen has proven promising for identifying low-dimensional materials and revealing new non-van der Waals candidates (see ref 40 for more details).

### Benchmarking

Before using FCDimen to classify dimensionalities, we must first ensure a reliable calculation of FCs. Loew et al. have shown that UMLIPs can predict phonon dispersion curves accurately,<sup>46</sup> with MACE<sup>49,50</sup> and MatterSim<sup>48</sup> performing the best. We therefore adopted these two UMLIPs for benchmarking (see Methods for details). Reference FCs were taken from the Phonon database,<sup>51</sup> which includes phonon



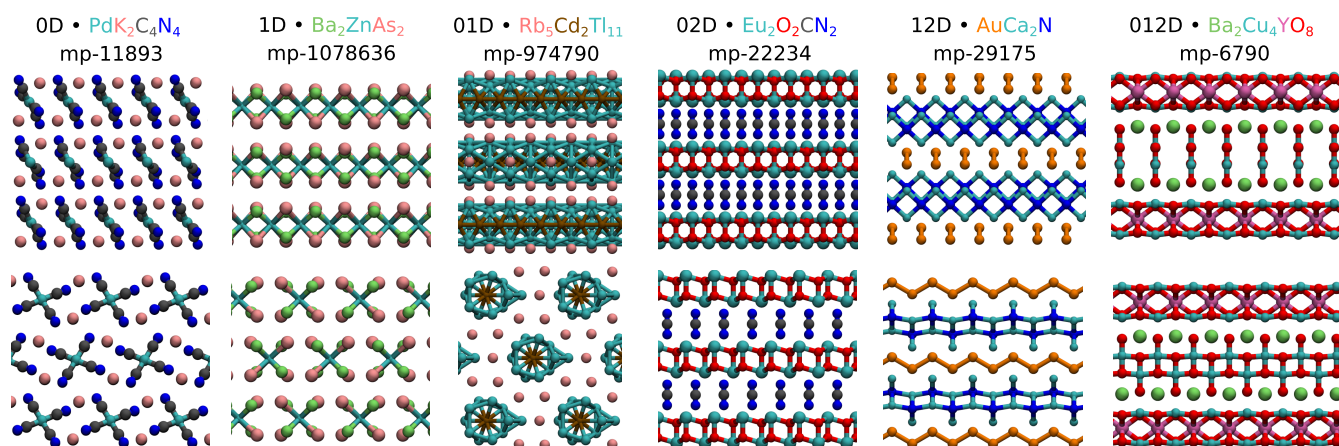
**Figure 1.** Validation of the methodology. Comparing DFT and ML (MatterSim) for (a) MaxFC and MinFC [eq 6], (b) distribution of MaxFC and MinFC, (c) maximum phonon frequencies at  $\Gamma$ -point, and (d) number of Phonon database structures in each dimensionality group. Panels (a) and (c) also show the related RMSE.



**Figure 2.** High-throughput calculation workflow and resulting dataset statistics. (a) Workflow for screening and high-throughput calculations. Each step indicates the number of structures involved. (b) Number of low-dimensional materials discovered in the screened dataset by FCDimen. “Other” corresponds to mixed dimensionalities with more than two types of dimensionalities (012D, 013D, and 023D). (c) Number of low-dimensional materials classified using the 16 most common space groups. (d) Heat map with occurrences of each element in low-dimensional materials in the dataset.

properties at the DFT level for 10,032 structures. This database was initially built using the PBEsol exchange-correlation functional. However, because both machine-

learning (ML) models were trained on data based on the PBE functional, a fair comparison required the use of Alexandria’s version of the Phonon database that was



**Figure 3.** Chemical structures of representative low-dimensional materials in the dataset (top and side views). Legends show the dimensionalities, chemical formulas, and MP IDs.

recalculated using the PBE functional.<sup>46</sup> For clean data and better comparisons, we applied the same screening criteria to the database as ref 40. Screening involved the following criteria: (i) enforcing a minimum supercell lattice constant of 5 Å; (ii) requiring that FCs at half the lattice distance remain below 20% of the MaxFC to ensure the supercell size was sufficient for FC decay; and (iii) filtering out chemically inert noble gases with negligible forces. Finally, we restricted our dataset to dynamically stable structures by excluding any materials exhibiting imaginary phonon frequencies (no imaginary phonon frequencies >0.1 THz) as determined by either DFT or ML. We compared only MaxFC and MinFC, not the entire FC matrix.

MatterSim predicted FCs accurately, with a root-mean-square error (RMSE) of 0.64 eV/Å<sup>2</sup> for MaxFC and 0.2 eV/Å<sup>2</sup> for MinFC (Figure 1a). MACE was slightly less accurate, with RMSEs of 0.86 and 0.34 eV/Å<sup>2</sup> (Supporting Information (SI) Figure S1a). The FC distributions for ML and DFT were very similar (Figures 1b and S1b). We remark that the RMSEs between PBE and PBEsol were even larger: 0.46 eV/Å<sup>2</sup> for MinFC and 0.99 eV/Å<sup>2</sup> for MaxFC (SI Figure S2a). Note that these correspond to relative errors of 5.5% for MaxFC and 9.2% for MinFC, which should ensure accurate predictions of the dimensionalities when combining UMLIPs with FCDimen.

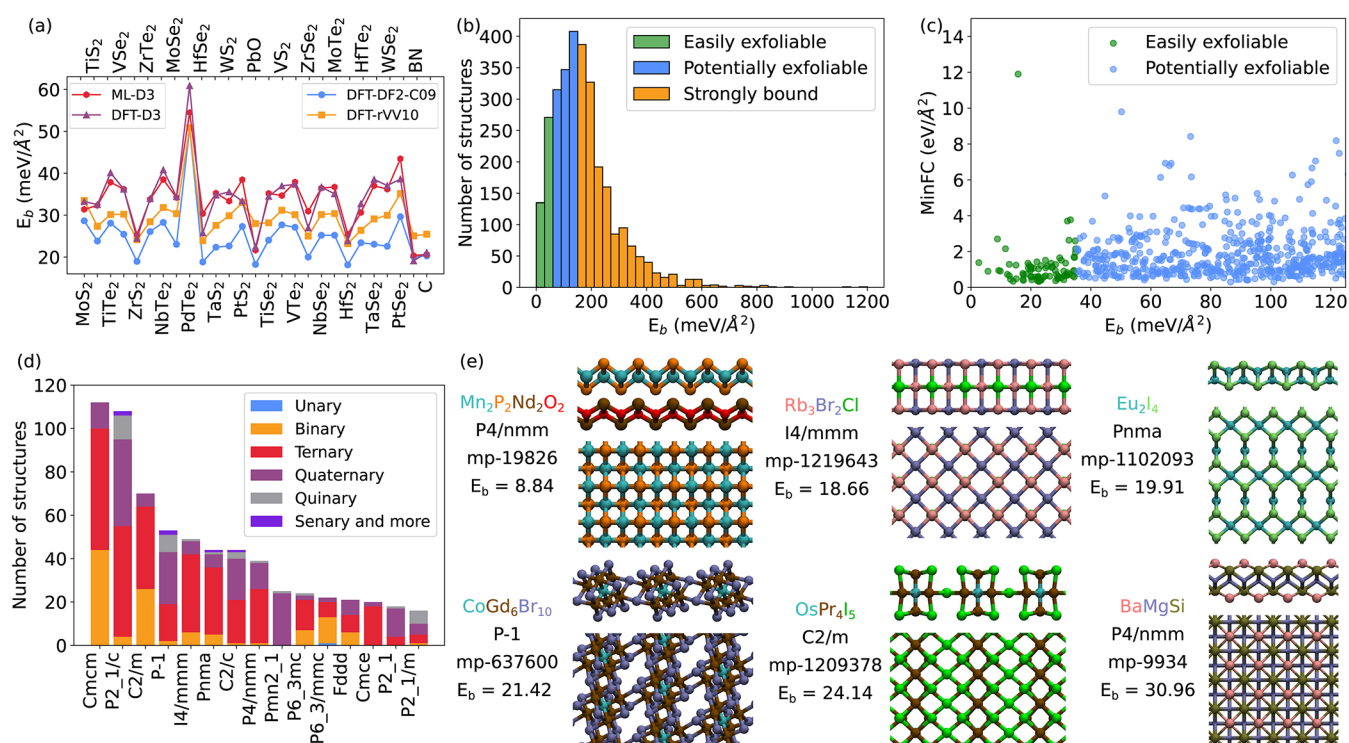
In addition to FCs, we also benchmarked FC-derived quantities, including the phonon frequencies and FCDimen dimensionality predictions. Phonon dispersions and frequencies had already been benchmarked by several UMLIPs, including MatterSim and MACE, which outperformed other UMLIPs.<sup>46</sup> Here, looking at the maximum phonon frequencies at the  $\Gamma$ -point, both ML models show excellent agreement with DFT, with RMSE of 0.57 THz for MatterSim (Figure 1c) and 0.76 THz for MACE (SI Figure S1c). ML-predicted dimensionalities were equally reliable. Out of the 4458 materials screened by the criteria of ref 40, MatterSim predicted dimensionalities correctly in 4021 (90.2%) cases (Figure 1d). MACE again performed slightly worse, with 3851 (86.4%) correct dimensionality predictions (SI Figure S1d). The agreement between PBE- and PBEsol-predicted dimensionalities was 90.0% (SI Figure S2b)—on par with MatterSim accuracy against PBE. Therefore, based on slightly better performance in predicting materials' FCs and their dimensionalities, we adopted MatterSim as our UMLIP of choice for further calculations.

### High-Throughput Calculations

Armed with a reliable UMLIP, we proceeded to carry out high-throughput calculations of FCs to discover low-dimensional materials in the Materials Project, an approach previously unfeasible due to the high cost of DFT calculations. The calculations were preceded by screening materials in the MP database (Figure 2a). We excluded materials having more than 100 atoms in the unit cell or elements unsupported by MatterSim, including noble gases and Tc, Lu, Po, At, and Yb. We also excluded materials containing Lu and La due to unreliable results. To direct our search toward stable and undiscovered low-dimensional materials, we further screened the dataset by the following steps: First, we removed materials already previously found to be low-dimensional, as identified by the method of Larsen et al.<sup>37</sup> As demonstrated in our previous work (ref 40), the materials identified as low-dimensional by conventional geometric descriptors were also found to be low-dimensional by FCDimen. Second, we removed materials included in the Phonon database since they had already been studied earlier by DFT and FCDimen.<sup>40</sup> Third, we removed theoretically predicted materials with energy above the convex hull ( $E_{\text{hull}}$ ) larger than 0.1 eV and experimentally observed materials with an  $E_{\text{hull}}$  larger than 0.2 eV based on MP data. This screening finally gave us 35,689 materials for the UMLIP-assisted high-throughput phonon calculations.

The phonon calculations gave 24,515 dynamically stable (no imaginary phonon frequencies >0.1 THz) materials. Analyzing these materials by FCDimen, we found 9139 low-dimensional materials including 3057 sheets (2D), 1760 chains (1D), 1838 clusters (0D), and 2484 mixed dimensionalities (Figure 2b). Materials with the highest dimensionality scores are presented in SI Tables S1–S4.

The discovered low-dimensional materials could be categorized into the 16 most common space groups, with *Pnma*, *P2<sub>1</sub>/c*, and *Cmcm* being the most common. In addition, binaries, ternaries, and quaternaries were the most commonly appearing species, which can be biased by the nature of the MP database (Figure 2c). Most materials contain metalloids (Ge and Si), reactive nonmetals (O, S, and P), and transition metals (Fe, Co, Ni) (Figure 2d). Promethium has the fewest compounds, and oxides dominate the materials, possibly because most of the materials in the MP are oxides.



**Figure 4.** Discovered 2D materials in detail. (a) Comparison of the binding energies of some known 2D materials calculated using ML (with D3–BJ damping) and DFT (DFT–D3, DF2–C09, and rVV10). DFT-calculated binding energies using DF2–C09 and rVV10 are taken from ref 27. (b) Number of 2D structures as a function of exfoliation energies using ML–D3–BJ. Structures are grouped into easily exfoliable ( $E_b \leq 35$  meV/Å<sup>2</sup>), potentially exfoliable ( $35 < E_b < 125$  meV/Å<sup>2</sup>), and strongly bound ( $E_b \geq 125$  meV/Å<sup>2</sup>) 2D materials. (c) Correlation between binding energies and MinFC for easily and potentially exfoliable 2D materials. (d) Easily and potentially exfoliable 2D materials categorized into 15 most common space groups. (e) Chemical structures (top and side views) of selected easily exfoliable 2D materials from the most common species (binary, ternary, and quaternary). Legends indicate space groups, chemical formulas, MP IDs, and binding energies ( $E_b$  values in meV/Å<sup>2</sup>).

Although low-dimensional units had mostly the same dimensionalities in a material, we also discovered mixed dimensionalities (Figure 3). Note that the geometry-based Larsen algorithm predicted all of these materials to be 3D bulk. The 0D units in these materials can take the form of either clusters or isolated atoms. In Rb<sub>2</sub>Cd<sub>2</sub>Tl<sub>11</sub>, for example, Cd<sub>2</sub>Tl<sub>11</sub> nanotubes are surrounded by rubidium atoms. These isolated atoms can be expected to form bulk Rb upon exfoliation. Moreover, in Eu<sub>2</sub>O<sub>2</sub>CN<sub>2</sub>, CN<sub>2</sub> molecules are intercalated between Eu<sub>2</sub>O<sub>2</sub> layers, creating a 02D dimensionality. In AuCa<sub>2</sub>N, 1D Au chains are intercalated between 2D Ca<sub>2</sub>N sheets, creating 12D dimensionality. Here, the behavior of the 1D gold chains during exfoliation is uncertain; they might either be stable or form 2D goldene or bulk gold. A few materials even contain three different dimensionalities. An example of such a material is Ba<sub>2</sub>Cu<sub>4</sub>YO<sub>8</sub> (Figure 3), which contains Cu<sub>2</sub>YO<sub>4</sub> layers, Cu<sub>2</sub>O<sub>4</sub> chains, and isolated barium atoms. For such a complex material, the products of the 1D and 0D units after exfoliation are unpredictable.

In addition, we identified 390 02D material candidates, 12 of which have dimensionality scores  $\geq 0.6$  and a high potential to be etched (SI Table S5). Finally, we identified 501 01D materials, 16 of them having dimensionality scores  $\geq 0.6$  (SI Table S6).

## 2D Materials in Detail

To investigate the discovered 2D materials in more detail, we calculated their interlayer binding energies  $E_b$ . We accounted for the weak van der Waals interactions by applying the D3 dispersion correction.<sup>63–66</sup> Recently, Sauer et al.<sup>67</sup> demon-

strated that UMLIPs with dispersion corrections are ready for large-scale structural simulations of 2D vdW material heterostructures, identifying MatterSim as one of the leading models in their evaluation. Consistent with these findings, we validated the reliability of ML–D3 calculations by benchmarking our results against DFT-calculated binding energies for a group of known 2D materials (Figure 4a). The binding energies from ML (D3–BJ damping) and DFT (D3–BJ, DF2–C09,<sup>27</sup> and rVV10<sup>27</sup>) agreed reasonably well. However, most of the D3–BJ binding energies (ML and DFT) were above those of the two other approaches due to the functional form or damping. We therefore selected our exfoliation energy thresholds slightly higher ( $\sim 5$  meV/Å<sup>2</sup>) than those in refs<sup>24,27,68</sup>.

We grouped the discovered 3057 2D materials into three categories based on  $E_b$ : easily exfoliable ( $E_b \leq 35$  meV/Å<sup>2</sup>), potentially exfoliable ( $35 < E_b < 125$  meV/Å<sup>2</sup>), and strongly bound ( $E_b \geq 125$  meV/Å<sup>2</sup>) (Figure 4b). Consequently, we found 183 easily exfoliable and 953 potentially exfoliable 2D materials. Apart from BN (mp-2653), all of the easily exfoliable materials had MinFC below 5 eV/Å<sup>2</sup> (Figure 4c).

The 2D materials are categorized into the 15 most common space groups, with *Cmcm*, *P2<sub>1</sub>/c*, and *C2/m* being the most prominent (Figure 4d). Figure 4e shows the chemical structures of the six selected 2D materials from the most common species (binary, ternary, and quaternary). We performed DFT phonon calculations for four nonmagnetic 2D materials and compared them with ML-predicted phonon dispersions (SI Figure S3). Although the agreement for these particular cases was not strong, it validated the accuracy of

UMLIPs in identifying true stability, consistent with ref 46. ML-predicted phonon dispersions of these selected 2D materials are shown in SI Figure S4. We compared the chemical structures, formulas, and materials IDs (if applicable) of the discovered 2D materials in known databases, including the computational two-dimensional database (C2DB),<sup>69,70</sup> materials cloud two-dimensional structure database (MC2D),<sup>27,68</sup> 2D MatPedia,<sup>71</sup> 2D topological insulators,<sup>72</sup> NOMAD (RAE database),<sup>73</sup> 2D charged building block databases (2DBBs),<sup>74</sup> and Materials Project.<sup>36,47</sup> We found 146 easily exfoliable (SI Table S7) and 741 potentially exfoliable 2D materials that could not be found in these databases.

## CONCLUSION

We demonstrated that both MACE and MatterSim predict interatomic force constants and material dimensionalities with an accuracy comparable to that of first-principles calculations. Using the slightly better-performing MatterSim, we calculated phonons for 35,689 Materials Project structures, kept the stable ones, and classified their dimensionalities using a method not based on geometries but on true chemical bonding between the atoms. Consequently, we discovered 9139 low-dimensional materials: 1838 clusters, 1760 chains, 3057 sheets, and 2484 mixed-dimensional systems. For the discovered 2D materials, we further calculated the interlayer binding energies and found that 146 are easily exfoliable and 741 are potentially exfoliable 2D materials. These 2D materials do not exist in known 2D materials databases. We believe that combining ML with the bond-strength-based dimensionality classification method will continue to help discover and explore low-dimensional materials for future applications. We also hope that our discovery inspires experimental work and leads to further expansion of the low-dimensional materials catalog.

## ASSOCIATED CONTENT

### Data Availability Statement

All data supporting the findings have been deposited in the databases at [10.5281/zenodo.17035156](https://doi.org/10.5281/zenodo.17035156).

### Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.chemmater.5c03151>.

Additional details on benchmark results of universal machine-learning interatomic potentials, a list of found low-dimensional materials with the highest score, sample Python scripts to facilitate the usage of databases, and phonon dispersion of selected 2D materials (PDF)

## AUTHOR INFORMATION

### Corresponding Authors

**Mohammad Bagheri** – Nanoscience Center, Department of Physics, University of Jyväskylä, 40014 Jyväskylä, Finland; [orcid.org/0000-0002-3501-2779](https://orcid.org/0000-0002-3501-2779); Email: [mohammad.m.bagheri@jyu.fi](mailto:mohammad.m.bagheri@jyu.fi)

**Pekka Koskinen** – Nanoscience Center, Department of Physics, University of Jyväskylä, 40014 Jyväskylä, Finland; [orcid.org/0000-0001-7711-3562](https://orcid.org/0000-0001-7711-3562); Email: [pekka.j.koskinen@jyu.fi](mailto:pekka.j.koskinen@jyu.fi)

## Authors

**Ethan Berger** – Department of Physics, Chalmers University of Technology, SE-41296 Gothenburg, Sweden; [orcid.org/0000-0001-9143-4493](https://orcid.org/0000-0001-9143-4493)

**Hannu-Pekka Komsa** – Microelectronics Research Unit, Faculty of Information Technology and Electrical Engineering, University of Oulu, FIN-90014 Oulu, Finland; [orcid.org/0000-0002-0970-0957](https://orcid.org/0000-0002-0970-0957)

Complete contact information is available at: <https://pubs.acs.org/doi/10.1021/acs.chemmater.5c03151>

## Notes

The authors declare no competing financial interest.

## ACKNOWLEDGMENTS

We acknowledge the Jane and Aatos Erkkö Foundation for funding (project EcoMet) and the Research Council of Finland for support under Academy Project No. 357483. The authors thank the EuroHPC Joint Undertaking for awarding this project access to the EuroHPC supercomputer LUMI, hosted by CSC (Finland) and the LUMI consortium through a EuroHPC Regular Access call. We also thank CSC–IT Center for Science Ltd. for generous additional grants of computer time.

## REFERENCES

- (1) Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; Firsov, A. A. Electric Field Effect in Atomically Thin Carbon Films. *Science* **2004**, *306*, 666–669.
- (2) Radisavljevic, B.; Radenovic, A.; Brivio, J.; Giacometti, V.; Kis, A. Single-Layer MoS<sub>2</sub> Transistors. *Nat. Nanotechnol.* **2011**, *6*, 147–150.
- (3) Butler, S. Z.; Hollen, S. M.; Cao, L.; et al. Progress, Challenges, and Opportunities in Two-Dimensional Materials Beyond Graphene. *ACS Nano* **2013**, *7*, 2898–2926.
- (4) Manzeli, S.; Ovchinnikov, D.; Pasquier, D.; Yazyev, O. V.; Kis, A. 2D Transition Metal Dichalcogenides. *Nat. Rev. Mater.* **2017**, *2*, No. 17033.
- (5) Xiang, R.; Inoue, T.; Zheng, Y.; et al. One-Dimensional Van der Waals Heterostructures. *Science* **2020**, *367*, 537–542.
- (6) Han, W.; Huang, P.; Li, L.; Wang, F.; Luo, P.; Liu, K.; Zhou, X.; Li, H.; Zhang, X.; Cui, Y.; Zhai, T. Two-Dimensional Inorganic Molecular Crystals. *Nat. Commun.* **2019**, *10*, No. 4728.
- (7) Du, L.; Zhao, Y.; Wu, L.; et al. Giant Anisotropic Photonics in the 1D Van der Waals Semiconductor Fibrous Red Phosphorus. *Nat. Commun.* **2021**, *12*, No. 4822.
- (8) Wei, N.; Tian, Y.; Liao, Y.; Komatsu, N.; Gao, W.; Lyuleeva-Husemann, A.; Zhang, Q.; Hussain, A.; Ding, E.-X.; Yao, F.; Halme, J.; Liu, K.; Kono, J.; Jiang, H.; Kauppinen, E. I. Colors of Single-wall Carbon Nanotubes. *Adv. Mater.* **2021**, *33*, No. 2006395.
- (9) Turunen, M.; Brotons-Gisbert, M.; Dai, Y.; Wang, Y.; Scerri, E.; Bonato, C.; Jöns, K. D.; Sun, Z.; Gerardot, B. D. Quantum Photonics with Layered 2D Materials. *Nat. Rev. Phys.* **2022**, *4*, 219.
- (10) Burch, K. S.; Mandrus, D.; Park, J.-G. Magnetism in Two-Dimensional Van der Waals Materials. *Nature* **2018**, *563*, 47–52.
- (11) Gibertini, M.; Koperski, M.; Morpurgo, A. F.; Novoselov, K. S. Magnetic 2D Materials and Heterostructures. *Nat. Nanotechnol.* **2019**, *14*, 408–419.
- (12) Klein, J.; Pingault, B.; Florian, M.; et al. The Bulk Van der Waals Layered Magnet CrSBr is a Quasi-1D Material. *ACS Nano* **2023**, *17*, 5316–5328.
- (13) Kim, S. J.; Koh, H.-J.; Ren, C. E.; Kwon, O.; Maleski, K.; Cho, S.-Y.; Anasori, B.; Kim, C.-K.; Choi, Y.-K.; Kim, J.; Gogotsi, Y.; Jung, H.-T. Metallic Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene Gas Sensors with Ultrahigh Signal-to-Noise Ratio. *ACS Nano* **2018**, *12*, 986–993.

- (14) Hosseini-Shokouh, S. H.; Zhou, J.; Berger, E.; Lv, Z.-P.; Hong, X.; Virtanen, V.; Kordas, K.; Komsa, H.-P. Highly Selective H<sub>2</sub>S Gas Sensor Based on Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene–Organic Composites. *ACS Appl. Mater. Interfaces* **2023**, *15*, 7063–7073.
- (15) Zhou, J.; Bagheri, M.; Järvinen, T.; Pravda Bartus, C.; Kukovec, A.; Komsa, H.-P.; Kordas, K. C<sub>60</sub>Br<sub>24</sub>/SWCNT: A Highly Sensitive Medium to Detect H<sub>2</sub>S via Inhomogeneous Carrier Doping. *ACS Appl. Mater. Interfaces* **2021**, *13*, 59067–59075.
- (16) Deng, D.; Novoselov, K. S.; Fu, Q.; Zheng, N.; Tian, Z.; Bao, X. Catalysis with Two-Dimensional Materials and Their Heterostructures. *Nat. Nanotechnol.* **2016**, *11*, 218–230.
- (17) Cho, Y. S.; Kang, J. Two-Dimensional Materials as Catalysts, Interfaces, and Electrodes for An Efficient Hydrogen Evolution Reaction. *Nanoscale* **2024**, *16*, 3936–3950.
- (18) Zhang, M.; Wang, Z.; Bo, X.; Huang, R.; Deng, D. Two-Dimensional Catalysts: From Model to Reality. *Angew. Chem., Int. Ed.* **2025**, *64*, No. e202419661.
- (19) Xie, M.; Tang, S.; Zhang, B.; Yu, G. Metallene-Related Materials for Electrocatalysis and Energy Conversion. *Mater. Horiz.* **2023**, *10*, 407–431.
- (20) Kou, L.; Ma, Y.; Sun, Z.; Heine, T.; Chen, C. Two-Dimensional Topological Insulators: Progress and Prospects. *J. Phys. Chem. Lett.* **2017**, *8*, 1905–1919.
- (21) Balandin, A. A.; Kargar, F.; Salguero, T. T.; Lake, R. K. One-Dimensional Van der Waals Quantum Materials. *Mater. Today* **2022**, *55*, 74–91.
- (22) Campi, D.; Kumari, S.; Marzari, N. Prediction of Phonon-Mediated Superconductivity with High Critical Temperature in the Two-Dimensional Topological Semimetal W<sub>2</sub>N<sub>3</sub>. *Nano Lett.* **2021**, *21*, 3435–3442.
- (23) Kezilebieke, S.; Huda, M. N.; Vaňo, V.; Aapro, M.; Ganguli, S. C.; Silveira, O. J.; Glodzik, S.; Foster, A. S.; Ojanen, T.; Liljeroth, P. Topological Superconductivity in A Van der Waals Heterostructure. *Nature* **2020**, *588*, 424–428.
- (24) Björkman, T.; Gulans, A.; Krasheninnikov, A. V.; Nieminen, R. M. Van der Waals Bonding in Layered Compounds from Advanced Density-Functional First-Principles Calculations. *Phys. Rev. Lett.* **2012**, *108*, No. 235502.
- (25) Lebègue, S.; Björkman, T.; Klintonberg, M.; Nieminen, R. M.; Eriksson, O. Two-Dimensional Materials from Data Filtering and Ab Initio Calculations. *Phys. Rev. X* **2013**, *3*, No. 031002.
- (26) Ashton, M.; Paul, J.; Sinnott, S. B.; Hennig, R. G. Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials. *Phys. Rev. Lett.* **2017**, *118*, No. 106101.
- (27) Mounet, N.; Gibertini, M.; Schwaller, P.; Campi, D.; Merkys, A.; Marrazzo, A.; Sohler, T.; Castelli, I. E.; Cepellotti, A.; Pizzi, G.; Marzari, N. Two-Dimensional Materials from High-Throughput Computational Exfoliation of Experimentally Known Compounds. *Nat. Nanotechnol.* **2018**, *13*, 246–252.
- (28) Lyngby, P.; Thygesen, K. S. Data-Driven Discovery of 2D Materials by Deep Generative Models. *npj Comput. Mater.* **2022**, *8*, No. 232.
- (29) Friedrich, R.; Ghorbani-Asl, M.; Curtarolo, S.; Krasheninnikov, A. V. Data-driven Quest for Two-Dimensional Non-Van der Waals Materials. *Nano Lett.* **2022**, *22*, 989–997.
- (30) Barnowsky, T.; Krasheninnikov, A. V.; Friedrich, R. A New Group of 2D Non-van der Waals Materials with Ultra Low Exfoliation Energies. *Adv. Electron. Mater.* **2023**, *9*, No. 2201112.
- (31) Barnowsky, T.; Timm, C.; Friedrich, R. Exfoliation and Cleavage of Crystals from a Universal Potential. **2025**.
- (32) Moustafa, H.; Larsen, P. M.; Gjerding, M. N.; Mortensen, J. J.; Thygesen, K. S.; Jacobsen, K. W. Computational Exfoliation of Atomically Thin One-Dimensional Materials With Application to Majorana Bound States. *Phys. Rev. Mater.* **2022**, *6*, No. 064202.
- (33) Bagheri, M.; Komsa, H.-P. Screening 0D Materials for 2D Nanoelectronics Applications. *Adv. Electron. Mater.* **2023**, *9*, No. 2200393.
- (34) Li, Y.; Wan, G.; Zhu, Y.; Yang, J.; Zhang, Y.-F.; Pan, J.; Du, S. High-Throughput Screening and Machine Learning Classification of Van der Waals Dielectrics for 2D Nanoelectronics. *Nat. Commun.* **2024**, *15*, No. 9527.
- (35) Khazaei, M.; Bae, S.; Khaledialidusti, R.; Ranjbar, A.; Komsa, H.-P.; Khazaei, S.; Bagheri, M.; Wang, V.; Mochizuki, Y.; Kawamura, M.; Cuniberti, G.; Allaei, S. M. V.; Ohno, K.; Hosono, H.; Raebiger, H. Superlattice MAX Phases with A-Layers Reconstructed into 0D-Clusters, 1D-Chains, and 2D-Lattices. *J. Phys. Chem. C* **2023**, *127*, 14906–14913.
- (36) Ganose, A. M.; Jain, A. Robocrystallographer: Automated Crystal Structure Text Descriptions and Analysis. *MRS Commun.* **2019**, *9*, 874–881.
- (37) Larsen, P. M.; Pandey, M.; Strange, M.; Jacobsen, K. W. Definition of A Scoring Parameter to Identify Low-Dimensional Materials Components. *Phys. Rev. Mater.* **2019**, *3*, No. 034003.
- (38) Cheon, G.; Duerloo, K.-A. N.; Sendek, A. D.; Porter, C.; Chen, Y.; Reed, E. J. Data Mining for New Two- and One-Dimensional Weakly Bonded Solids and Lattice-Commensurate Heterostructures. *Nano Lett.* **2017**, *17*, 1915–1923.
- (39) Gorai, P.; Toberer, E. S.; Stevanović, V. Computational Identification of Promising Thermoelectric Materials Among Known Quasi-2D Binary Compounds. *J. Mater. Chem. A* **2016**, *4*, 11110–11116.
- (40) Bagheri, M.; Berger, E.; Komsa, H.-P. Identification of Material Dimensionality Based on Force Constant Analysis. *J. Phys. Chem. Lett.* **2023**, *14*, 7840–7847.
- (41) Deringer, V. L.; Caro, M. A.; Csányi, G. Machine Learning Interatomic Potentials as Emerging Tools for Materials Science. *Adv. Mater.* **2019**, *31*, No. 1902765.
- (42) Behler, J. Four Generations of High-Dimensional Neural Network Potentials. *Chem. Rev.* **2021**, *121*, 10037–10072.
- (43) Jinnouchi, R.; Minami, S. Machine Learning Force Fields in Electrochemistry: From Fundamentals to Applications. *ACS Nano* **2025**, *19*, 22600–22644.
- (44) Riebesell, J.; Goodall, R. E. A.; Benner, P.; Chiang, Y.; Deng, B.; Ceder, G.; Asta, M.; Lee, A. A.; Jain, A.; Persson, K. A. A Framework to Evaluate Machine Learning Crystal Stability Predictions. *Nat. Mach. Intell.* **2025**, *7*, 836–847.
- (45) Berger, E.; Bagheri, M.; Komsa, H.-P. Screening of Material Defects using Universal Machine-Learning Interatomic Potentials. *Small* **2025**, *21*, No. e03956.
- (46) Loew, A.; Sun, D.; Wang, H.-C.; Botti, S.; Marques, M. A. L. Universal Machine Learning Interatomic Potentials Are Ready for Phonons. *npj Comput. Mater.* **2025**, *11*, No. 178.
- (47) Jain, A.; Ong, S. P.; Hautier, G.; Chen, W.; Richards, W. D.; Dacek, S.; Cholia, S.; Gunter, D.; Skinner, D.; Ceder, G.; Persson, K. A. Commentary: The Materials Project: A Materials Genome Approach to Accelerating Materials Innovation. *APL Mater.* **2013**, *1*, No. 011002.
- (48) Yang, H.; Hu, C.; Zhou, Y. et al. MatterSim: A Deep Learning Atomistic Model Across Elements, Temperatures and Pressures. **2024**.
- (49) Batatia, I.; Kovacs, D. P.; Simm, G. N. C.; Ortner, C.; Csányi, G. *Advances in Neural Information Processing Systems*; Oh, A. H.; Agarwal, A.; Belgrave, D.; Cho, K., Eds.; Curran Associates, Inc., **2022**.
- (50) Batatia, I.; Batzner, S.; Kovács, D. P.; Musaelian, A.; Simm, G. N. C.; Drautz, R.; Ortner, C.; Kozinsky, B.; Csányi, G. The Design Space of E(3)-Equivariant Atom-Centered Interatomic Potentials. *Nat. Mach. Intell.* **2025**, *7*, No. 1.
- (51) Togo, A.; Tanaka, I. First Principles Phonon Calculations in Materials Science. *Scr. Mater.* **2015**, *108*, 1–5.
- (52) Chen, C.; Ong, S. P. A Universal Graph Deep Learning Interatomic Potential for the Periodic Table. *Nat. Comput. Sci.* **2022**, *2*, 718–728.
- (53) Larsen, A. H.; Mortensen, J. J.; Blomqvist, J.; et al. The Atomic Simulation Environment—A Python Library for Working with Atoms. *J. Phys.:Condens. Matter.* **2017**, *29*, 273002.
- (54) Bitzek, E.; Koskinen, P.; Gähler, F.; Moseler, M.; Gumbusch, P. Structural Relaxation Made Simple. *Phys. Rev. Lett.* **2006**, *97*, No. 170201.

(55) Ong, S. P.; Cholia, S.; Jain, A.; Brafman, M.; Gunter, D.; Ceder, G.; Persson, K. A. The Materials Application Programming Interface (API): A Simple, Flexible and Efficient API for Materials Data Based on Representational State Transfer (REST) Principles. *Comput. Mater. Sci.* **2015**, *97*, 209–215.

(56) Ong, S. P.; Richards, W. D.; Jain, A.; Hautier, G.; Kocher, M.; Cholia, S.; Gunter, D.; Chevrier, V. L.; Persson, K. A.; Ceder, G. Python Materials Genomics (pymatgen): A Robust, Open-Source Python Library for Materials Analysis. *Comput. Mater. Sci.* **2013**, *68*, 314–319.

(57) Togo, A.; Shinohara, K.; Tanaka, I. Spglib: A Software Library for Crystal Symmetry Search. *Sci. Technol. Adv. Mater.:Methods* **2024**, *4*, No. 2384822.

(58) Togo, A.; Chaput, L.; Tadano, T.; Tanaka, I. Implementation Strategies in Phonopy and Phono3py. *J. Phys.:Condens. Matter* **2023**, *35*, 353001.

(59) Togo, A. First-Principles Phonon Calculations with Phonopy and Phono3py. *J. Phys. Soc. Jpn.* **2023**, *92*, No. 012001.

(60) Kresse, G.; Furthmüller, J. Efficiency of Ab-Initio Total Energy Calculations for Metals and Semiconductors using a Plane-Wave Basis Set. *Comput. Mater. Sci.* **1996**, *6*, 15–50.

(61) Kresse, G.; Furthmüller, J. Efficient Iterative Schemes for Ab Initio Total-Energy Calculations using a Plane-Wave Basis Set. *Phys. Rev. B* **1996**, *54*, 11169–11186.

(62) Blöchl, P. E. Projector Augmented-Wave Method. *Phys. Rev. B* **1994**, *50*, 17953–17979.

(63) Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the Damping Function in Dispersion Corrected Density Functional Theory. *J. Comput. Chem.* **2011**, *32*, 1456–1465.

(64) Grimme, S. Semiempirical GGA-Type Density Functional Constructed with A Long-Range Dispersion Correction. *J. Comput. Chem.* **2006**, *27*, 1787–1799.

(65) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010**, *132*, 154104.

(66) Takamoto, S.; Shinagawa, C.; Motoki, D.; et al. Towards Universal Neural Network Potential for Material Discovery Applicable to Arbitrary Combination of 45 Elements. *Nat. Commun.* **2022**, *13*, No. 2991, DOI: 10.1038/s41467-022-30687-9.

(67) Sauer, M. O.; Lyngby, P. M.; Thygesen, K. S. Dispersion-Corrected Machine Learning Potentials for 2D Van der Waals Materials. *Phys. Rev. Mater.* **2025**, *9*, 074007.

(68) Campi, D.; Mounet, N.; Gibertini, M.; Pizzi, G.; Marzari, N. Expansion of the Materials Cloud 2D Database. *ACS Nano* **2023**, *17*, 11268–11278.

(69) Haastrup, S.; Strange, M.; Pandey, M.; Deilmann, T.; Schmidt, P. S.; Hinsche, N. F.; Gjerding, M. N.; Torelli, D.; Larsen, P. M.; Riis-Jensen, A. C.; Gath, J.; Jacobsen, K. W.; Jørgen Mortensen, J.; Olsen, T.; Thygesen, K. S. The Computational 2D Materials Database: High-Throughput Modeling and Discovery of Atomically Thin Crystals. *2D Mater.* **2018**, *5*, No. 042002.

(70) Gjerding, M. N.; Taghizadeh, A.; Rasmussen, A.; et al. Recent Progress of the Computational 2D Materials Database (C2DB). *2D Mater.* **2021**, *8*, No. 044002.

(71) Zhou, J.; Shen, L.; Costa, M. D.; Persson, K. A.; Ong, S. P.; Huck, P.; Lu, Y.; Ma, X.; Chen, Y.; Tang, H.; Feng, Y. P. 2DMPedia, An Open Computational Database of Two-Dimensional Materials from Top-Down and Bottom-Up Approaches. *Sci. Data* **2019**, *6*, No. 86.

(72) Marrazzo, A.; Gibertini, M.; Campi, D.; Mounet, N.; Marzari, N. Relative Abundance of Z<sub>2</sub> Topological Order in Exfoliable Two-Dimensional Insulators. *Nano Lett.* **2019**, *19*, 8431–8440.

(73) Evans, M. L.; Bergsma, J.; Merkys, A.; et al. Developments and Applications of the OPTIMADE API for Materials Discovery, Design, and Data Exchange. *Digital Discovery* **2024**, *3*, 1509–1533.

(74) Deng, J.; Pan, J.; Zhang, Y.-F.; Du, S. Database Construction of Two-Dimensional Charged Building Blocks for Functional-Oriented Material Design. *Nano Lett.* **2023**, *23*, 4634–4641.



CAS INSIGHTS™

## EXPLORE THE INNOVATIONS SHAPING TOMORROW

Discover the latest scientific research and trends with CAS Insights. Subscribe for email updates on new articles, reports, and webinars at the intersection of science and innovation.

Subscribe today

**CAS**  
A division of the  
American Chemical Society