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High-throughput prediction of novel two-dimensional materials
NICOLAS MOUNET, PHILIPPE SCHWALLER, ANDREA CEPELLOTTI, Ecole Polytechnique Federale de Lausanne, Switzerland, ANDRIUS MERKYS, Vilnius University, Lithuania, IVANO ELIGIO CASTELLI, MARCO GIBERTINI, GIOVANNI PIZZI, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne, Switzerland — As a crucial step towards the identification of novel and promising 2D materials, we provide here a large scale first-principles exploration and characterization of such compounds. More than 300,000 three-dimensional structures from several crystallographic databases are screened systematically by checking the absence of chemical bonds between adjacent layers, identifying close to 5,000 layered systems. Then DFT calculations of the van der Waals interlayer bonding are performed with automatic workflows, while systematically assessing the metallic, insulating or magnetic character of the materials obtained. Following full atomic and cell relaxations, phonon dispersions are computed as a first step towards the assessment of thermodynamic properties. Thanks to the AiiDA materials' informatics platform [1], and in particular its automatic workflow engine, database structure, sharing capabilities, and pipelines to/from crystallographic repositories, the systematic and reproducible calculation of these properties becomes straightforward, together with seamless accessibility and sharing. [1] G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari and B. Kozinsky, Comp. Mat. Sci. 111, 218 (2016).

Nicolas Mounet
EPFL, Switzerland

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