Saulėtekio Puslaidininkių Fizikos Seminaras



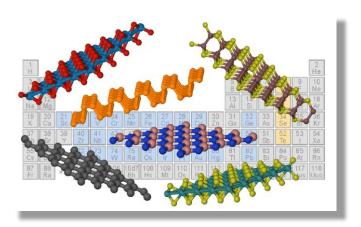


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High-throughput materials discovery: The Computational 2D Materials Database

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An big interest in the field of 2D materials has emerged in recent years due to their unique properties and applications. *The Computational 2D Materials Database* sets a new paradigm in predicting novel 2D materials from *ab-initio* calculations, with a balance between the number of predicted materials and the range of their properties included in the database. The details of this high-throughput approach will be presented. As of now the database contains more than 3000 materials, and properties are described at different levels of complexity, from the stability analysis to the electronic structure of excited states.



