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Hybrid *ab initio*-machine learning simulations of dislocations.

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Abstract:

Dislocations are extended line defects which carry plastic deformation in crystalline materials. Understanding and optimizing dislocation behaviour by characterising dislocation interaction with point defects is a central topic in computational metallurgy. For this task, *ab initio* calculations, specifically density functional theory (DFT), are essential to capture dislocation core structures and complex bonding to impurity elements. However, the computational cost of DFT typically has cubic scaling with the number of atoms for metallic systems, which limits its direct applicability to the study of extended defects. In this seminar I will present how hybrid QM/MM methods in combination with modern machine learning force fields allow to study unfeasibly large systems with *ab initio* accuracy.

Short bio:

I am from Saint-Petersburg, Russia and obtained my master degree in Physics from Peter the Great St. Petersburg Polytechnic University in 2012. The same year I enrolled in a Ph.D. program shared between Ghent University and Complutense University of Madrid within the framework of Erasmus Mundus FUSION-DC. However I spent most of my time at Belgian Nuclear Research Centre SCK•CEN in Mol, Belgium working on my research project together with Structural Materials expert group.

I defended my Ph.D. in April 2017 and, shortly after that, joined Warwick Centre for Predictive Modelling as a Research Fellow. In December 2020 I started as a postdoc at the Départment Théorie et Simulation Numérique of Centre Interdisciplinaire de Nanoscience de Marseille (CINaM). You can find more details about my career path and research projects at my personal page: https://pgrigorev.github.io/.