DE LA RECHERCHE À L'INDUSTRIE

cea

Séminaire

SRMP

Mercredi 20 mars 2013 à 10h30

Salle de réunion du SRMP – Bâtiment 520 - Pièce 109

Analytic bond-order potentials for modelling iron and its alloys

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In iron and many iron-based alloys the magnetic energy represents a significant contribution to the binding energy. An interatomic potential for the simulation of iron alloys therefore needs to include an adequate description of magnetism. In this talk I present the derivation of a magnetic interatomic potential that is suitable for simulating millions of atoms. The potential is obtained by systematically coarse graining the electronic structure from density functional theory through tight-binding to the bond-order potentials. I show that the resulting potential includes non-collinear magnetism and may be further simplified to a Ginzburg-Landau description of magnetism. Analytic expressions for forces and torques will be presented. Applications of the potential to modelling Fe, Fe-C and Mn will be discussed.

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