

Lundi 17 Juin 2019 à 10h30

Salle de réunion du SRMP – Bâtiment 520 - Pièce 109

Multiscale QM/MM Modeling of Materials Chemomechanics

James Kermode

Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick

Fracture and plasticity are the dominant failure processes underlying many materials reliability issues. They are also some of the most challenging multiscale modelling problems, requiring both an accurate description of chemical processes occurring near crack tips or dislocation cores and the inclusion of much larger model systems. These requirements can be met simultaneously by combining quantum mechanical descriptions of chemically active regions with classical atomistic models that capture the long-range elastic behaviour of the surrounding crystal matrix, using approaches such as the 'Learn on the Fly' (LOTF) scheme. I will review recent methodological advances that: (i) improve the efficiency of the scheme using machine learning and identify remaining limitations with uncertainty quantification approaches; (ii) extend to rare events by computing minimum energy paths in multiscale systems; (iii) extend to metallic systems. Together, these enable processes such as dislocation motion in the presence of impurities to be described.

Les visiteurs de nationalité étrangère hors Union Européenne sont priés de bien vouloir avvertir **3 semaines à l'avance**, et ceux de l'Union Européenne **5 jours ouvrés** avant le séminaire, le Secrétariat du Service de leur entrée sur le Centre : Tel : 01 69 08 66 64 – mail : patricia.matysiak@cea.fr

Commissariat à l'énergie atomique et aux énergies alternatives
DEN/DANS/DMN Service de Recherches de Métallurgie Physique
Centre de Saclay – Bât. 520 - 91191 Gif-sur-Yvette Cedex – France