LABEX CAPRYSSES

Post-doctoral position available	
Job title	Post-doctoral fellowship in computational materials science https://euraxess.ec.europa.eu/jobs/721554
General information	Workplace: GREMI (Orléans, France) Contract period: 12 months Starting date: May 2021 Candidate must submit a Curriculum Vitae, a motivation letter, a copy of the PhD diploma including jury report, a copy of ID card or passport and 2 reference letters. Applications must be sent by e-mail to Dr Pascal Brault pascal.brault@univ-orleans.fr
Missions	The postdoctoral researcher will conduct numerical simulations, at molecular scales, erosion of relevant materials mimicking debris erosion during atmospheric re-entry. She/He will conduct suitable molecular simulations using advanced computing resources.
Activities	The study of wake interaction phenomena is one of the problems that must be taken into account when dealing with the atmospheric re-entry of space debris such as satellites or spacecraft boosters, because it has a strong influence on their trajectory and impact location [1-2]. Under certain conditions, the fall of space debris passing through the dense atmospheric phase, where high temperatures are reached, ends with its complete or partial destruction due to fragmentation and ablation. During ablation phenomena, aerothermodynamics of space debris will change modifying the wake structure. In addition to aerodynamic aspects, this process will produce dust and particles that will contribute in part to the accumulation of aerosol particles present from the ground to the upper atmosphere (~100 km). The origin is mainly due to dust coming from comets, and from the meteoritic disintegration but a quantity becoming each year more important provides from artificial debris. From an environmental point of view, dust play a major role in the radiative balance of the Earth's atmosphere and thus in climate, and in chemical processes such as those destroying the stratospheric ozone layer. Molecular Dynamics simulations will be carried out for describing elementary processes of erosion under these conditions [3]. Basically, Molecular dynamics simulations calculated the full trajectories of a set of particles. The only required ingredients are the force fields describing the interactions. Fortunately, two classes of force-fields are now available for describing reactivity of materials in extreme conditions: reaxFF and COMB3 forcefields [4,5]. They will provide accurate erosion rates and shapes, molecules and radicals formation rates in the vicinity of the debris surface. On the other hand, even functional form of force fields is existing, not all materials composition is parametrized for allowing direct molecular dynamics simulations. In this context, two ways will be explored: parametrizing the force field with known properties and/or using quantum chemistry approach which directly couple molecular dynamics to density functional Theory (DFT) [6]. The latter is used for accurately calculating interactions between species at each step of the molecular dynamics run. This provides a robust way for treating any relevant system, but at the expense of high CPU cost. These will be compared with the experimental results from PHEDRA facility for a deeper understanding of the erosion processes and will enable to predict debris evolution and dust composition in the atmosphere. **Références** : [1] Space debris: the ESA approach, 7th Eur. Conf. Space Debris, ESA/ESOC Darmstadt (GERMANY), 18-21 april 2017. [2] W. Ailor, W. Hallman, G. Steckel, M. Weaver, Analysis of re-entered debris and implications for survivability modeling, Proc. 4th Eur. Conf. Space Debris, ESA. 2005, 587. [3] D. Graves and P. Brault, Molecular dynamics for low temperature plasma-surface interaction studies, J. Phys. D 42 (2009) 194011 [4] Tao Liang et al, Reactive Potentials for Advanced Atomistic Simulations, Annu. Rev. Mater. Res. 2013. 43:109–29 [5] E. Neyts, P. Brault, Molecular dynamics simulations for plasma surface interactions, Plasma Processes and Polymers 14 (2017) 1600145

	[6] A. Michalak, T. Ziegler, Modeling Chemical Reactions with First-Principle Molecular Dynamics, in Molecular Materials with Specific Interactions – Modeling and Design, W. A. Sokalski Ed., Springer Netherlands, 2017 pp. 225-274
Skills	The candidate should hold a PhD in the field of computational material science with emphasis on chemical and surface reactivity in the field of materials erosion in extreme conditions. Extensive practice of reactive molecular dynamics and skills on DFT and DFT coupled to MD are required. Published articles as main author are expected. • Additional knowledge on plasma erosion of materials will be appreciated. • Fluent English both written and spoken is mandatory. Fluent French speaking is advised. • Ease to write articles, reports and presenting results at conferences and during project reviews is expected.
Context of the work	GREMI (CNRS, Université d'Orléans) has a long expertise, both experimental and with molecular simulations, in plasma. Computational resources are available at GREMI and at CASCIMODOT computing center. LAMMPS software and AMS suite from SCM company will be available for DFT/DFT-MD simulations.
Supplementary information	The closing date for receiving applications is January, 31st 2022. The selection procedure is in 2steps: First, selecting a short list of best candidates and second, the final selection after an hearing.