Three years position at SRMP and SGLS, University Paris-Saclay, CEA: Advancing Materials Science through Machine Learning

A three-year position is open at the *Section de Recherches de Métallurgie Physique* (SRMP) and the *Service de Génie Logiciel pour la Simulation* (SGLS) at CEA Paris-Saclay, starting in March 2024. SRMP is a part of Department of Research on Materials and Physical Chemistry (DRMP), which is responsible for understanding and advancing knowledge in physico-chemical processes related to material science and engineering in extreme environments and for low-carbon energy applications. The SRMP, Physical Metallurgy Research Section of Service of Corrosion and Material Behavior Research (S2CM) , specializes in materials science, bringing together theoretical, numerical, and experimental approaches and leveraging them with AI-based methods in order to address the challenges in nuclear and renewable energy innovations.

SGLS on the other hand, is a part of the *Département de Modélisation des Systèmes et des Structures* (DM2S), which is in charge of developing simulation tools to design systems in the core disciplines of nuclear research. As such, the SGLS has a number of missions: to provide data processing tools to interact with calculation softwares, to develop HPC computation platforms and offer expertise in numerical analysis applied to neutronics, mechanics and thermohydraulics, to promote AI in numerical simulation and implement methods to measure uncertainties of research studies carried out by physicians.

Scientific context and goals. Statistical methods, such as Machine Learning (ML) trained on physical data, can prove invaluable when traditional approaches face limitations or encounter obstacles, such as high computational costs. The candidate will develop and implement cutting-edge methods utilizing the open-souce MiLaDy (Machine Learning Dynamics) package [1, 2]. Key responsibilities will include the integration and expansion of MiLaDy by connecting it with various packages and platforms from materials science community to enhance the functionality and performance of the code. Here are a few examples of previous work that will be improved upon: (i) Combining ML with accelerated Molecular Dynamics based on the Bayesian adaptive biasing force method [2] to sample the complex energy landscapes of defects. (ii) Providing reliable force fields capable of handling radiation-induced defects in materials [1] (iii) Exploring the atomistic free energy landscape of metals with *ab initio* accuracy up to the melting temperature [3]. (iv) Proposing surrogate models to bypass traditional approaches for accessing challenging properties, such as vibrational entropies [4]. Great attention will be devoted to the database design to ensure robust performance of ML approaches for materials science applications.

Required skills. We are seeking a motivated candidate with a PhD in computational materials science, physics, or a related discipline, skilled and passionate with programming . Familiarity with HPC languages such as C++ and/or Fortran is highly advantageous. Previous experience in the development of Machine Learning/Deep Learning protocols is a plus but not required.

How to apply. Please send your application, including a motivation letter and a complete CV with references we may contact, to Mihai-Cosmin Marinica (mihai-cosmin.marinica@cea.fr), Alexandra Goryaeva (alexandra.goryaeva@cea.fr) and Anida Khizar (anida.khizar@cea.fr). The deadline for applications is December 30, 2023.

References:

[1] A. M. Goryaeva *et al.* Nature Commun. **14**, 3003 (2023); A. M. Goryaeva *et al.* Nature Commun. **11**, 4691 (2020);
[2] M.-C. Marinica, A. M. Goryaeva, *et al*, MiLaDy - Machine Learning Dynamics, CEA Saclay, 2015-2023: https://ai-atoms.github.io/milady/ ;
[3] A. Zhong, C. Lapointe, A. M. Goryaeva, J. Baima, M. Athènes, and M.-C. Marinica,, Phys. Rev. Mater. **7**, 023802 (2023);
[4] C. Lapointe, *et al.* , Phys. Rev. Materials **4**, 063802 (2020); C. Lapointe, *et al*, Phys. Rev. Materials **6**, 113803 (2022).