POLITECNICO DI MILANO

PhD in INGEGNERIA DEI MATERIALI / MATERIALS ENGINEERING - 38th cycle

PARTENARIATO PNRR Research Field: MULTISCALE MODELING & ENGINEERING APPLICATIONS

Monthly net income of PhDscholarship (max 36 months)
€ 1325.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	Among the emerging technological challenges certainly the development of solutions for environmentally friendly, and sustainable, energy production, transportation and utilization is at the center of great research efforts. The development of multiscale models, which combine information coming from the atomic scale to the macroscopic scale, can play a key role in enabling new technologies in the energy sector. In particular the focus of this research will be in the development of computational methodologies that allow to model systems of interest using models that combine first principle and molecular dynamics simulations. The developed computational methodology will be used to investigate systems of interest for engineering applications. As an example, a system that may be investigated is electric energy storage. Batteries and fuel cells are based on materials that can reversibly store ions and/or undergo controlled redox reactions. Here, the development of new materials with optimal properties is a very active research field. For instance, the membranes that separate the cathode and the anode in hydrogen fuel cells constitute a key element that determines the performance and long-term behavior of the device. Similarly, the lithium storage capacity of graphitic anodes in Li ion batteries determines the battery capacity, which ultimately sets the range of electric vehicles. By improving the overall understanding of the basic features that determine the behavior of materials in batteries or fuel cells one may hope to

	overcome current limitations and provide guidelines for the development of better materials that may lead to increased device performance. This challenge encompasses phenomena occurring at different scales (e.g., molecular/atomic level in the case of reactions, molecular/morphological level in the case of ion diffusion), and it can be undertaken properly through a multiscale approach. The outcome would be an effective model by which, e.g., the lithium storage capacity of graphite anodes or the gas permeability in fluorinated polymeric membranes for fuel cells, could be optimized by tuning in-silico the structure of the materials.
Methods and techniques that will be developed and used to carry out the research	The computational methodologies that will be developed will consist both in quantum mechanical atomistic models that provide the key parameters governing chemical reactions and interatomic interactions at the microscopic level, and molecular dynamics methods that may employ this low-level information to determine the behavior of the materials at a much larger scale. Currently available quantum chemical methods (QM) can provide a reliable and realistic description of the mentioned atomistic phenomena. Similarly, current molecular dynamics codes (MM) may be very effective in providing information about the interplay between molecular structure and morphological behavior – which ultimately governs diffusion phenomena in polymeric materials. To connect the two scales (QM/MM) one has to properly define the system and the set of effective QM parameters that have to be fed into the MM code. Because of the complexity of the systems to be investigated, and because of the required number of calculations to be executed for statistical significance, the QM/MM interface cannot be handled by human inspection and operation. The setup of sets of QM calculations, collection of parameters and data feeding into the MM code should be orchestrated by a computer code, which will be developed and written on purpose during the PhD project. The developed computational strategy will be used to investigate systems of interest for the energy sector. For example, in the case of study of energy storage, it may be applied to study lithium-ion storage and diffusion in nanostructured carbon

	materials for anodes in batteries, or gas permeability and chemical stability of fuel cell membranes.
Educational objectives	Understanding and using autonomously the available computer codes for quantum chemistry and molecular dynamics. Mastering the use of HPC facilities, including the optimal use of the available resources, the programming of codes for molecular modeling, data processing and analysis.
Job opportunities	PhD students with skills in molecular modeling of materials and data analysis may find occupation in chemical industries or companies that develop new functional materials as well as in process industries.
Composition of the research group	1 Full Professors 2 Associated Professors 1 Assistant Professors 1 PhD Students
Name of the research directors	Tommasini-Raffaini-Cavallotti

Contacts
https://www4.ceda.polimi.it/manifesti/manifesti/controller/ricerche/RicercaPerDocentiPublic.do?evn_didattica=evento&k_doc=38352&polij_device_category=DESKTOP&__pj0=0&__pj1=7d73cd0916a937eb5332010d7703501f *https://www4.ceda.polimi.it/manifesti/manifesti/controller/ricerche/RicercaPerDocentiPublic.do?evn_didattica=evento&k_doc=162754&polij_device_category=DESKTOP&__pj0=0&__pj1=79a678caef469edb7ccd0a56b41b69ec* *https://www4.ceda.polimi.it/manifesti/manifesti/controller/ricerche/RicercaPerDocentiPublic.do?evn_didattica=evento&k_doc=135717&polij_device_category=DESKTOP&__pj0=0&__pj1=4ebd36c276a625bef2e202d108eb2171*

Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	662.5 €
By number of months	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
The candidate will have to fill in a mandatory questionnaire in order to close the application. **Individual budgetfor research** (during the 3 years): about 5.400 euro **Teaching assistantship**: availability of funding in recognition of supporting teaching activities by the PhD student. There are various forms of financial of for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.