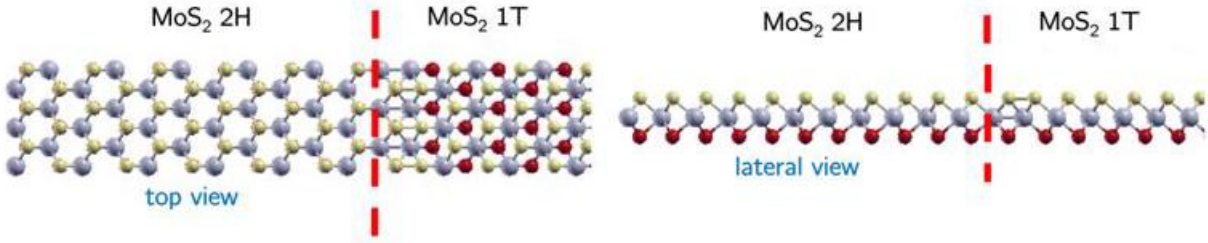
1 ESR position available on: « Quantum Simulations of 2D Heterostructures »

Location: National Research Council (CNR), Pisa (Tuscany), Italy.
Time frame: Start around October 2019 – 1 year term, renewable up to 3 years

1 ESR position is available funded by a FET-Open project: "Quantum Engineering for Machine Learning" (acronym: QUEFORMAL) within the call: H2020-FETOPEN-01-2018-2019-2020. The topic is Quantum Mechanical (QM) simulations supporting fabrication and engineering of devices combining hetero-structures of 2-dimensional materials (2DMs) into low-voltage field-effect transistors and non-volatile memories.

- **Scientific context**

The FET-Open project QUEFORMAL[1] involves 2 theory groups (CNR, Pisa, Italy, and University of Pisa, Italy, coordinator), 2 experimental groups (EPFL, Lausanne, Switzerland, and University of Bundeswehr-München, Germany), and 2 European SMEs (AMO, http://www.amo-gmbh.com/en/, and Quantavis, http://www.quantavis.com/). The final goal of QUEFORMAL is to develop a novel transport technology based on 2D heterostructures. The CNR unit will deal with first-principles atomistic simulations of materials and devices based on 2D lateral and vertical heterostructures. The targets are: (i) to provide QM-derived data on such materials and interfaces to be fed into higher-level models thus allowing predictive simulations of phase transformation and transport phenomena. and ii) to shed light on the atomistic origin of fundamental materials properties to guide materials design.



- **Related Publications :**
  - Katagiri et al. “Gate-tunable atomically-thin lateral MoS2 Schottky junction patterned by electron beam”, Nano Letters Vol. 16 (6), pp. 3788-3794, 2016
  - Cusati et al. “Electrical properties of graphene-metal contacts”, Scientific Reports, Vol. 7(1), art. no. 5109, 2017
  - Oxide Materials at the Two-Dimensional Limit (Springer, Germany, 2016, http://www.springer.com/fr/book/9783319283302) Springer series in materials science (vol. XVII), DOI: 10.1007/978-3-319-28332-6.

We are looking for a motivated early-stage researcher, with interest and knowledge on 2D materials. Salary is 17160 €/year (net). Expertise in density-functional theory (DFT) for structure and electronic band structure prediction and transport simulation (e.g., QuantumEspresso suite of codes) is a pre-requisite. Applications (including reference persons) should be sent via email to:

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[1] https://ec.europa.eu/digital-single-market/en/news/european-innovation-council-pilot-invest-eu124-million-38-new-high-risk-innovative-projects
[2] http://www.researchgate.net/profile/Alessandro_Fortunelli/, http://www.pi.iccom.cnr.it/ThC2-Lab