



Physics, Accuracy and Machine Learning: Towards the next generation of Molecular Potentials.

11 PhD positions are available in the Marie Skłodowska-Curie Doctoral Network

PHYMOL brings together leading experts in the fields of molecular simulations, quantum chemistry, crystal structure prediction, intermolecular modelling, spectroscopy, machine-learning, and nano-clusters, from 12 academic institutes & laboratories, and 4 industrial entities, in an ambitious programme of research and training to develop a new generation of researchers in the field of molecular modelling.

Available projects

1. [DC1: Towards the accurate description of the induction energy in SAPT](#)
2. [DC2: Intermolecular interactions in excited states: the CO–CO* and other excimers](#)
3. [DC3: Collision-induced absorption and high-resolution spectra calculated from ab initio potentials](#)
4. [DC4: Reparametrisation of semiempirical models](#)
5. [DC5: Development of intermolecular force-fields with many-body dispersion interactions](#)
6. [DC6: Consistent treatment of polarization and charge-delocalization in many-body systems](#)
7. [DC7: How intermolecular interactions shape polymorphic energy landscapes](#)
8. [DC8: State-of-the art modelling of new quantum materials: surface-supported metal atomic quantum clusters](#)
9. [DC9: Implicit machine-learning solvent models for confined spaces.](#)
10. [DC10: Adapting state-of-the-art modelling of new quantum materials to industry-standard open-source big data analysis tools.](#)
11. [DC11: Density-mapped FFs: Rapid prototyping of force-fields based on physical and ML mappings onto the electronic density](#)

For project details and also details of the recruitment process go to the PHYMOL webpage (<https://phymol.eu/>). **Projects are either 36 or 48 months in duration.**

Benefits

- Cutting-edge science in an international collaboration in the UK/EU/US.
- Generous remittance: 1) *Living allowance* of €3,400 (country correction coefficient applies), 2) *Mobility allowance* of €600, 3) *Family allowance* (€660), if applicable. Employer costs and other deductions depend on the recruiting organisation.

Requirements & Eligibility

- International applicants with a strong interest in the scientific goals of PHYMOL.
- Applicants should hold a MSc or equivalent degree in the field of physics, chemistry, or chemical engineering.
- Experience & keen interest in programming (Python/C++/Fortran) is essential.
- **MSCA Mobility Rule:** Researchers must not have resided or carried out their main activity (work, studies, etc.) in the country of the host organisation for more than 12 months in the 3 years immediately before the recruitment date. Exceptions apply. *This rule may mean that you cannot apply for some projects.*
- Further eligibility requirements and the selection process are described on our [recruitment page](#).

How to apply?

- The application process is described on our Recruitment page (<https://phymol.eu/recruitment.php>)
- We are accepting pre-applications immediately.
- Initial application deadline: **01.03.2023**
- Candidates will be enrolled between **15.03.2023** to **01.09.2023**

Contacts

In case of any inquiries about open positions and recruitment, please contact us via this email: phymol@umk.pl Further information about PHYMOL, our scientific goals, and all participants can be found on our website: <https://phymol.eu/>

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Project Manager: Ms Agata Wiśniewska (a_wis@umk.pl)



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