Annex 05 – MOSES

Scientific-Disciplinary Sector:	CHEM-02/A Physical Chemistry
Contract duration (max 24 months):	24 months
Profile of the researcher to be hired:	• Interdisciplinary skills in theoretical chemistry, scientific programming, and computational simulations. • Experience with *ab initio* methods and molecular dynamics for the study of complex systems. • Knowledge of computational chemistry software for advanced simulations. • Proficiency in Fortran (recommended), C/C++, and Python. • Experience in parallelization (MPI, OpenMP, CUDA) for computational optimization. • Competence in code management using Git/GitHub and Zenodo.
Description of the research project the postdoctoral researcher will be involved in:	The project aims to investigate new catalytic reactions in the context of sustainable chemistry and to design innovative green materials. In particular, the project will focus on the development of advanced theoretical and computational methodologies in physical chemistry, using *ab initio* techniques such as density functional theory (DFT) and molecular dynamics simulations. Both adiabatic and non-adiabatic approaches (Born-Oppenheimer and Surface Hopping) will be employed to model complex chemical environments, including liquid phases, solvents, polymeric and protein matrices. A central aspect of the project will be the optimization of computational performance through the implementation of parallelization techniques (MPI, OpenMP). A graphical user interface will be developed for simulation setup and data post-processing.