Postdoctoral position in Computational Materials Design

A **one-year** postdoctoral position in **computational materials design of crystalline solids** is offered at the *Molecular Materials Theoretical Chemistry* group of the *Institute of Molecular Science* (Valencia, Spain). The position is framed within the "*Molecular Electronics Devices*" research line of the Excellence Unit María de Maeztu CEX2019-000919-M grant funded by MCIN/AEI/10.13039/501100011033. The average gross salary is of **2200** €/month, and the contract can be **extended for an additional year**.

The candidate will apply quantum chemistry methods (mainly density functional theory) and big-data techniques to non-conventional perovskite-type materials in order to discover new compositions that allow performance improvement and lower environmental impact with respect to the archetypal lead-halide perovskite. The thermodynamics of chemical modification and formation of defects will be analysed in detail for the three-dimensional bulk material and the low-dimensional counterparts (0D, 1D and 2D). The structure and electronic effects of the boundaries between crystalline grains and the interface with other materials (hole/electron transport layers), will be thoroughly characterized towards application in hybrid perovskite solar cells or solid-state, light-emitting LED devices.

Requirements:

- PhD degree in Materials Science, Chemistry, Physics or related field.
- Expertise in computational modelling of solid-state systems.
- Good programming skills and Linux management.
- Good verbal and written communication skills in English.

Interested candidates should contact one of the principal investigators of the project, Dr. Joaquín Calbo (joaquin.calbo@uv.es) or Prof. Enrique Ortí (enrique.orti@uv.es), at the earliest with the following information:

(i) A cover letter highlighting their interest in the position.
(ii) Curriculum vitae.
(iii) The names and contact addresses (e-mail) of two academic referees.

The successful applicant is expected to start between September and December 2022.