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## RECURSOS HUMANOS – CONVOCATÒRIA DE VACANT

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### Postdoctoral position in computational catalysis

#### ■ DESCRIPCIÓ DEL LLOC DE TREBALL / JOB POSITION DESCRIPTION

- Study the catalytic processes involved in alkane dehydrogenation on single atom catalyst and reactivity on bimetallic cluster catalysts.
- Identify and enumerate geometrical and electronic topological descriptors that could help designing in-silico new catalyst materials.
- Assess the use of a reactive force field in the study of heterogeneous-catalyzed reactions enabling the handling of more realistic models.

#### ■ PERFIL DE LA PERSONA CANDIDATA /PROFILE OF THE CANDIDATE

- Doctor/PhD

#### ■ REQUISITS/REQUISITES

- Background in computational chemistry with experience in periodic DFT calculations.
- Background in machine learning techniques.
- Programming skills.
- Fluency in written and oral English, and strong, written, oral communication skills.

#### ■ ES VALORARÀ / IT WILL BE CONSIDERED

- Familiar with reactive force fields.
- Familiar with catalysis modelling.
- Interest in continuous improvements of processes by integrating innovative solutions.
- Ability to work as a team member, as well as independently with minimal supervision.
- Reference letters are welcome.

#### ■ CONDICIONS LABORALS / LABORAL CONDITIONS

- Jornada complet / Full time position
- Ubicació del lloc de treball / Laboratory: [Group of Quantum Chemistry](#), [Inorganic and Physical Chemistry Dpt.](#), [Univ. Rovira i Virgili](#), Tarragona
- Contracte d'obra i servei / Contract for a specific project or service
- Durada/ Duration: 1 +1 year extension in function of the completion of the objectives
- Retribució / Gross salary: 2.200 € per month
- Incorporació / Starting data: April 2020

#### ■ SEND CV to A/e: [rrhh@fundacio.urv.cat](mailto:rrhh@fundacio.urv.cat) & [josep.ricart@urv.cat](mailto:josep.ricart@urv.cat)

Applications will be considered until the position is filled