

ICB seminar series 2019/20

chairman: Prof. Dr. Paolo Arosio

VOLCANOS, CLIFFS AND WAYS AROUND: STRATEGIES TO BREAK LINEAR SCALING RELATIONSHIPS IN CATALYSIS

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Abstract: The search for new catalytic materials has relied in highly time consuming procedures. The appearance of theoretical methods that employ Density Functional Theory coupled to kinetic models has allowed the rational understanding of activity volcano plots and selectivity abrupt profiles that resemble cliffs. However, these methodologies present several drawbacks as the optimization is confined to a family of materials and the maximum activity might not be enough for practical applications. Volcanos emerge from the symmetry between the adsorption energies of different intermediates on the catalyst and thus circumventing these dependencies is crucial to identify better catalytic materials. I present a revision of the advances in the field indicating that complexity in the materials is crucial to allow alternative paths and thus overcome the drawbacks of scaling-relationships and how artificial intelligence techniques will enhance rational catalytic design.

Bio: Núria López graduated in Chemistry and got her PhD degree in Theoretical Chemistry (1999) at the University of Barcelona, Spain (1995). She spent a postdoctoral period the Center for Atomic-scale Materials Physics led by Prof. Jens K. Nørskov (Denmark). In 2005 she started her independent carrier at ICIQ. Her research group focuses on the theoretical research heterogeneous photo-electro-catalysis. Prof. López has co-authored over 200 scientific publications. In 2010 she was awarded an ERC Starting Grant and then a ERC Proof-of-concept to allow open data and machine learning. She was awarded a “Prize for Excellence” by the Real Sociedad Española de Química. She has collaborated with several industries in Europe to leverage atomistic modeling, participated in 7 EU projects and served in several committees in EU. Currently she chairs the Scientific Steering Committee of the Supercomputing initiatives in Europe.