

CHEMICAL ENGINEERING

SEMINAR SERIES



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Hindered translator/rotor model to determine adsorbate entropy with DFT

ABSTRACT: Surface chemistry plays an important role in a large range of applications and technologies, especially in catalysis and electrocatalysis, separations, and device fabrication through film growth. Due to its technological relevance, a tremendous effort has been made worldwide to determine and predict reactions rates and selectivity for networks of elementary surface reactions through microkinetic modeling. Entropy plays an important part in kinetic pre-exponentials and equilibrium constants and for heterogeneous catalysis these are the entropy of adsorbates. We have developed an easy to implement method to calculate entropy of adsorbates using standard DFT approaches. Instead of solely using vibrational frequencies and the harmonic oscillator approximation to calculate all modes of motion in the partition function, we use a hindered translator and hindered rotor model for the three modes of motion parallel to the surface. This model joins the two limiting cases for adsorbates on a surface, the 2D ideal lattice gas model and the 2D ideal gas model, making it valid over large temperature range and for a variety of adsorbates. To verify this model, density functional theory was used to calculate adsorbate entropies of four different adsorbate species and found to agree well with experimental results. This method has been implemented into free computational tools, ASE and CatMAP, making it widely available.

RECEPTION 3:30 • LECTURE 4:00 – 5:00
PHYSICS ASTRONOMY BLDG. PAA A 118

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BIOGRAPHY: Líney Árnadóttir received her B.S. degree in Chemistry from the University of Iceland in 2001 and her PhD. in Chemical Engineering from the University of Washington Seattle in 2007 with Prof. Eric Stuve and Hannes Jónsson after which she joined Prof. Dave Castner and Lara Gamble for a postdoc in surface characterization. She joined the School of CBEE at Oregon State University as Assistant Professor in Fall 2012. Her research focuses on fundamental catalysis and surface engineering to enable technologies for a cleaner and safer planet through application of electronic structure calculations, kinetic theory development and surface science experiments.