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Department of Chemistry

Special Seminar

2 p.m. Friday, November 16, 2012 • 401/402 Walter Library

Professor

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Storage and Activation of Methane–ab initio approach

His research has explored the application of quantum chemical ab initio methods and the use of molecular modelling in chemistry, notably in the area of the structure, dynamics and reactivity of solid catalysts including zeolites and transition metal oxides.

Website: http://www.chemie.hu-berlin.de/forschung/quantenchemie/Group/js-1/js_cv

Abstract

Storage and activation of the energy-carrying molecules methane and hydrogen in metal-organic frameworks (MOF) is considered. Rational materials design requires knowledge of adsorption isotherms. A method for the ab initio prediction of adsorption isotherms is presented which relies on a multi-site Langmuir model and the calculation of equilibrium constants for individual sites by quantum chemistry and molecular statistics [1]. This way, information on the contribution of each type site as well as on adsorbate-adsorbate interactions which are included using the Bragg-Williams model are obtained [2]. This knowledge is key to a rational materials design. We apply a quantum chemical multilevel method (Hybrid MP2:PBE+D+ΔCCSD(T)) which is shown to yields adsorption energies with chemical accuracy (4 kJ/mol) [3].

The raw materials change from crude oil to natural gas and other carbon resources has renewed the interest in C-H bond activation of methane. We study the activation of C-H bonds on oxide materials in two different ways that are relevant for the oxidative coupling of methane to ethane: (i) H abstraction at oxygen radical sites on Li-doped and MgO [4,5] and (ii) heterolytic splitting on morphological (corner sites) and electronic (F centers) defects of MgO.

[1] K. Sillar, A. Hofmann, J. Sauer, J. Am. Chem. Soc. 131 (2009) 4143.
[2] K. Sillar, J. Sauer, J. Am. Chem. Soc. (2012) DOI 10.1021/ja307076t.
[3] S. Tosoni, J. Sauer, Phys. Chem. Chem. Phys. 12 (2010) 14330.
[4] K. Kwapien, M. Sierka, J. Döbler, J. Sauer, ChemCatChem 2 (2010) 819.
[5] S. Feyel, J. Döbler, R. Höckendorf, M.K. Beyer, J. Sauer, H. Schwarz, Angew. Chem., Int. Ed. 47 (2008) 1946, Angew. Chem. 120 (2008) 1972-1976.

Host: Professor Laura Gagliardi