BEP-relations for N2 dissociation over stepped transition metal and alloy surfaces - DTU Orbit (03/10/2019)

**BEP-relations for N2 dissociation over stepped transition metal and alloy surfaces**

We present density functional theory (DFT) calculations for N(2) dissociation on stepped face-centred cubic (211) surface slabs. By using the same crystal structure, the same adsorption site for atomic nitrogen, and the same transition-state bond length of N(2) over a range of pure metal surfaces, a perfectly linear Bronsted-Evans-Polanyi (BEP) relation between the transition-state potential energy and the dissociative chemisorption energy is obtained. The perfect BEP relation, which extends over 12 eV in chemisorption energy, suggests that the manifestation of BEP relations for surface reactions is a general electronic structure effect, and that geometric effects are responsible for the scatter which is normally observed around the BEP line. The BEP relation is also shown to be valid for both surface and bulk alloys. The scatter is, however, larger than for the pure elements. This can be understood as a larger geometrical variance. To analyze the accuracy of the DFT calculations a detailed convergence study is performed for several adsorbates on stepped hexagonal close-packed and face-centred cubic Ru slabs.

**General information**

Publication status: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Department of Chemistry, Center for Nanoteknologi, Centre for Catalysis and Sustainable Chemistry
Pages: 5202-5206
Publication date: 2008
Peer-reviewed: Yes

**Publication information**

Journal: Physical Chemistry Chemical Physics
Volume: 10
Issue number: 34
ISSN (Print): 1463-9076
Ratings:
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.166 SNIP 1.178
Web of Science (2008): Indexed yes
Original language: English
DOIs: 10.1039/b720021h
Source: orbit
Source ID: 232663
Research output: Contribution to journal › Journal article – Annual report year: 2008 › Research › peer-review