

CURRICULUM VITAE

Hannes Jónsson

Adjunct Professor of Chemistry (Research)

Education:

B.S. Chemistry, 1980 Univ. of Iceland;
Ph.D. Chemistry, 1985 Univ. of California San Diego;
Professor of Chemistry, Univ. of Washington;
Professor of Chemistry, Univ. of Iceland;
Visiting professor, Technical Univ. of Denmark;
Adjunct Professor of Chemistry, Brown Univ.

Theoretical physical chemistry: Development of methods for predicting the properties of chemicals and materials, in particular the mechanism and rate of transitions such as chemical reactions, diffusion, crystal growth, adsorption and desorption.

Research program:

The rapid advance in computers continues to open up new and exciting research possibilities in computational science. In the Jónsson group, theoretical methods are being developed and applied to computational studies of condensed matter to learn about the properties of liquids, crystals and amorphous solids in terms of the electronic wavefunctions and the atomic ordering and dynamics. Surfaces and interfaces have been a particular focus including the interaction of atoms and molecules with surfaces of solids. **For more information**, see <http://www.hi.is/~hj/researchprojects.html>

Recent Publications:

G. Henkelman, A. Arnaldsson and H. Jónsson, 'Theoretical calculations of CH₄ and H₂ associative desorption from Ni(111): could subsurface hydrogen play an important role?', J. Chem. Phys., vol. 124, p. 044706 (2006).

G. Henkelman, A. Arnaldsson and H. Jónsson, 'A fast and robust algorithm for Bader decomposition of charge density', Comp. Mat. Sci. 36, 354 (2006).

E. R. Batista, P. Ayotte, A. Bilic, B. D. Kay and H. Jónsson, 'What Determines the Sticking Probability of Water Molecules on Ice?', Phys. Rev. Letters, vol. 95, 223201 (2005).

L. Xu, G. Henkelman, C. T. Campbell and H. Jónsson, 'Small Pd clusters, up to the tetramer at least, are highly mobile on the MgO(100) surface', Phys. Rev. Letters, vol 95, page 146103 (2005).

R. M. Van Ginhoven, L. R. Corrales and H. Jónsson, 'Silica glass structure generation for ab initio calculations', Phys. Rev. B vol. 71, 024208 (2005).

T. Bligaard and H. Jónsson, 'Optimization of hyperplanar transition states: Application to 2D test problems', *Comp. Phys. Commun.*, vol. 169, p. 284 (2005).

R. A. Olsen, G. J. Kroes, G. Henkelman, A. Arnaldsson and H. Jónsson, 'Comparison of methods for finding saddle points without knowledge of the final states', *J. Chem. Phys.* vol. 121, 9776 (2004).

For a more complete list of publications,
see <http://www.hi.is/~hj/publications.html>

For the 'complete CV' link, use the URL
<http://www.hi.is/~hj/CVbrief.html>