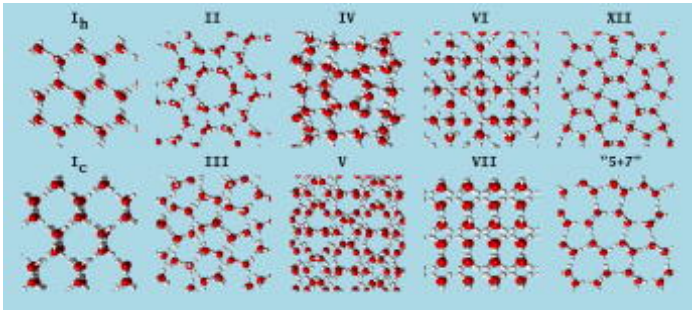
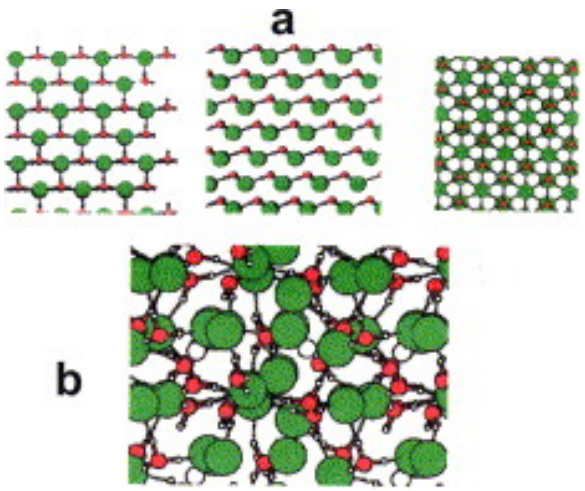
Remembering Victoria: Recent Work

1. Crystal structure using small unit cells

VB, R. Martonak, M. Parrinello *J. Chem. Phys*. **123**, 051108 (2005)
VB, R. Martonak, M. Parrinello *J. Chem. Phys*. **124**, 204705 (2006)

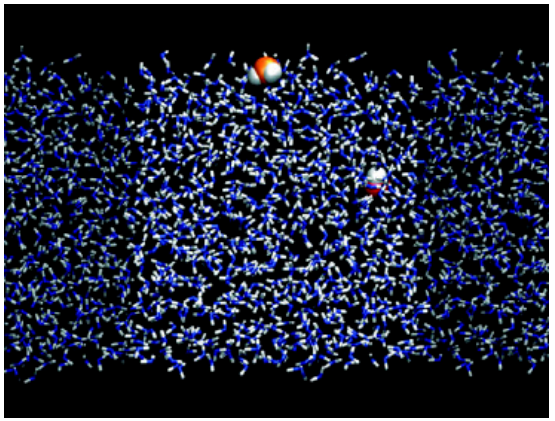


2. Hydrates of HCl (AIMD and FTIR)



J. P. Devlin, VB, F. Mohammed, M. Parrinello *Chem. Phys. Lett*. **432**, 362 (2006)
VB, F. Mohammed, M. Parrinello, J. P. Devlin *J. Chem. Phys*. **126**, 021102 (2007)
VB, F. Mohammed, M. Parrinello, J. P. Devlin *J. Chem. Phys*. **126**, 074503 (2007)
VB, A. Dubrovskiy, F. Mohammed, M. Parrinello, J. Sadlej, A. D. Hammerich, J. P. Devlin, *J. Phys. Chem. A* **112**, 2144 (2008)

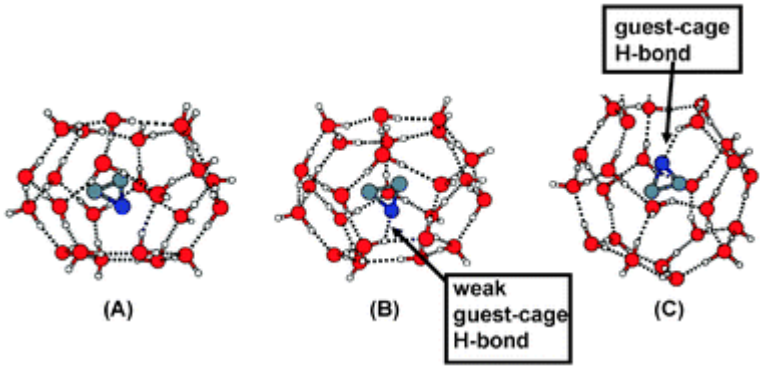
3. Aqueous interfaces.



"Water surface is acidic" VB, A. Millet, R. Vacha, P. Jungwirth, J. P. Devlin
Proc. Natl. Acad. Sci. **104**, 7342 (2007)
"Autoionization at the surface of neat water: Is the top layer pH neutral, basic, or acidic?"
R. Vacha, VB, A. Millet, J. P. Devlin, P. Jungwirth *Phys. Chem. Chem. Phys*. **9** (2007)
Comment by J. K. Beattie: *Phys. Chem. Chem. Phys*. **10**, 330 (2008)
Authors respond: *Phys. Chem. Chem. Phys*. **10**, 332 (2008)
"Surface of neat water is basic" J. K. Beattie *et al*. *Faraday Disc*. **141**, 31 (2009)

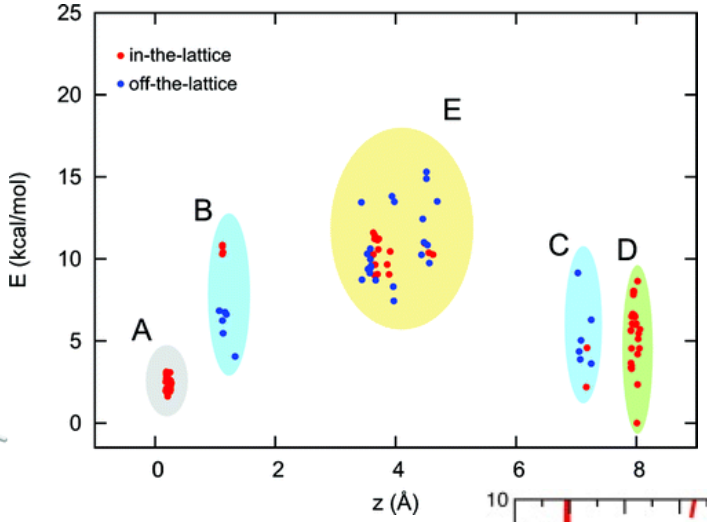
4. Clathrate hydrates

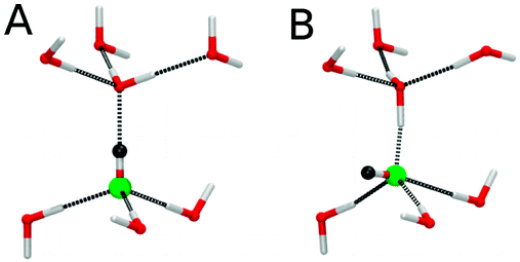
VB, J. P. Devlin, I. A. Monreal, B. Jagoda-Cwiklik, N. Uras-Aytemiz, L. Cwiklik *Phys. Chem. Chem. Phys*. **11** (2009)

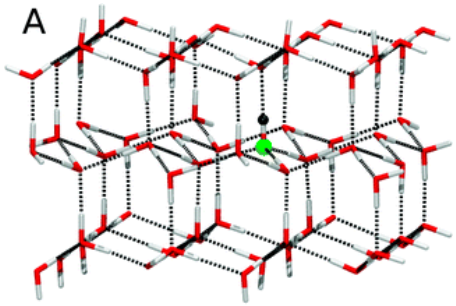


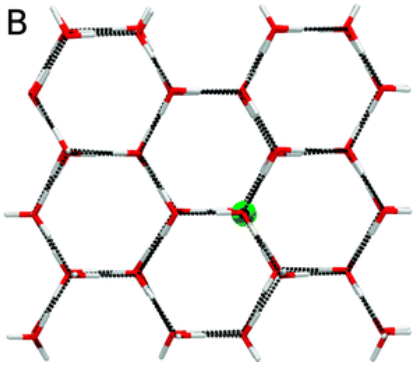
5. Hydroxide in ice.

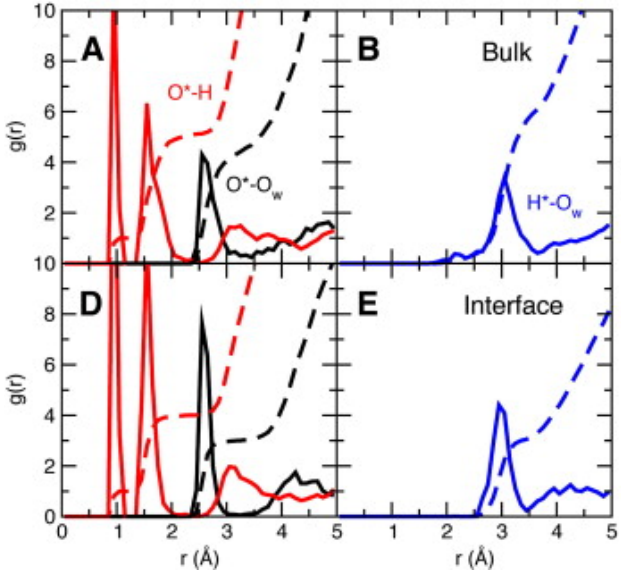
L. Cwiklik, VB Phys. Chem. Chem. Phys. 11, 1294 (2009)
L. Cwiklik, J. P. Devlin, VB J. Phys. Chem. A 113, 7482 (2009)

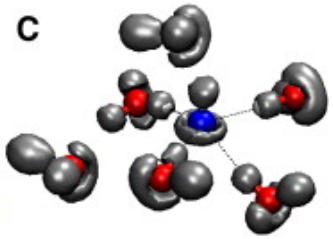


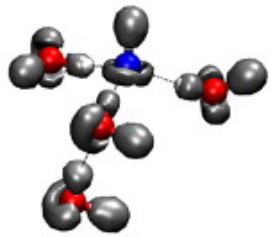












From Mundy *et al*. *Chem. Phys. Lett*. **481**, 2 (2009)

ידישעס ליד א

לאמיר הייבן נאך א פלאש דיר זו
זאגען יתגדל ויתקדש ון
אז דו ביסט געווייַן א גרויסע מענטש
זאלסט זיון אין אייביקייט געבענשט
די ארבעט וועט זיכער איסהאלטן
דו אבער וועשט אונדז דאך פעלן