

German Ab Initio Paper 1 May 2011

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German Ab Initio Paper 1
On the 21st of January 2009, I drove my car into my yard, and parked it just outside my house. Typical for northern Sweden in January, it was cold and snowy outside, and so I left my car engine running as I listened to the tail end of a radio programme. The programme consisted of a panel of 'experts' who discussed President Barack Obama's first inaugural address.

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Ab initio simulations are carried out at 300 K in the frameworks of metadynamics sampling and thermodynamic integration to map the thermal mechanisms of zwitterionization using Gly(H2O)_n with n = 4 and 10. In both cases, a similar water-mediated proton transfer chain mechanism is observed; yet, detailed analyses of thermodynamics and kinetics ...

Unveiling Zwitterionization of Glycine in the ...
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