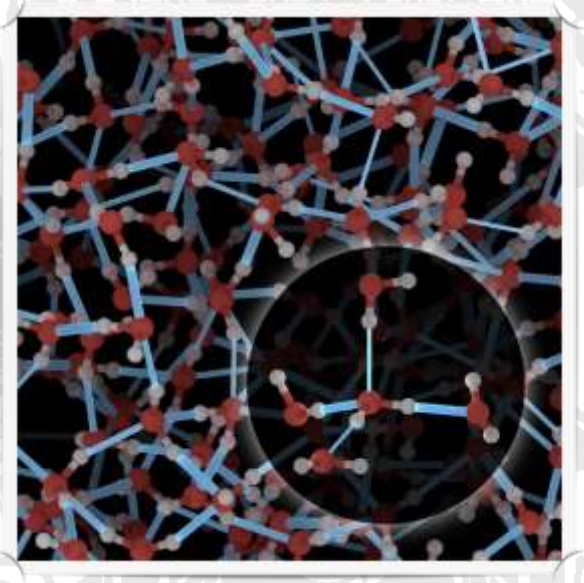
SONDERKOLLOQUIUM

AM 28. MÄRZ 2017 UM 09:00 UHR
IM SEMINARRAUM, GUSTAV-MIE-HAUS



The name is bond – Hydrogen bond

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A new energy decomposition analysis method for periodic systems based on absolutely localized molecular orbitals is presented [1, 2]. In combination with an accurate and efficient technique to compute nuclear quantum effects and the previously developed second generation Car-Parrinello molecular dynamics approach [3-5], this not only allows for quantum molecular dynamics simulations on previously inaccessible time and length scales, but also provide unprecedented insights into the nature of hydrogen bonding between water molecules. The effectiveness of this new combined approach is demonstrated on liquid water, ice and the water/air interface [6, 7]. Our simulations reveal that although a water molecule forms, on average, two strong donor and two strong acceptor bonds, there is a significant asymmetry in the energy of these contacts. We demonstrate that this asymmetry is a result of small instantaneous distortions of hydrogen bonds and show that the distinct features of vibrational and X-ray absorption spectra originate from molecules with high instantaneous asymmetry [8, 9]. Moreover, we found a striking correlation between the covalency of a hydrogen bond and the anisotropy of the proton magnetic shielding tensor, which enables to experimentally determine the strength and charge transfer of hydrogen bonding by NMR [10].

References
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