Abstract Submitted
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Dynamical investigation of water clusters in atmospheric conditions FRANCESCA BALETTO, King's College London, London WC2R 2LS, UK, MAL-SOON LEE, UGUETTE F.T NDONMGOUO, SANDRO SCANDOLO, ICTP, Trieste I-34014, Italy — Addressing environmental challenges via first principle calculations is one of the most promising subjects of numerical simulations. Here, we investigate the dynamical evolution of water clusters, namely the dimer and the hexamer, which are abundant in our atmosphere. We use these two clusters as prototypes to clarify long-standing dilemma of greenhouse effects and ozone depletion. To begin with, I will show the behavior of HCl on water hexamers [1]. Our calculations show that at zero temperature the most energetically favorable structure is obtained when the HCl is completely dissociated. At temperatures T $\sim$ 200 K, the vibrational entropic effects stabilize the non-dissociated clusters. This behavior is traced back to the large dynamic effects associated with the flexibility of the planar cluster. Water vapor absorption in the far-infrared region accounts a large portion of the total radiative absorption responsible for the greenhouse effect. We found that at T close to 200K, the dimer dynamics is fully anharmonic and the calculated adsorption strength throughout the far-infrared spectra is smaller than the measured vapor absorption continuum [2].
[1] U.F.T. Ndomgouo et al. JPCA accepted
[2] M-S. Lee, et al. submitted

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