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First Principles Study on Orientational Defects in Ice Ih: Effect of Adsorbates

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Orientational, Bjerrum, defects in ice are the intrinsic property and believed that the reason of proton conductivity in ice [1]. In this study, energy of formation and dynamics of the Bjerrum defects were investigated in the presence of small adsorbates, such as dimethyl ether, CO2 etc.. The main tool of this investigation is ab initio molecular dynamics as implemented in the density functional code QUICKSTEP [2] which is part of CP2K package [3]. A crystal slab of three bilayers of hexagonal ice containing 72 water molecules were used as a model. The energy cost for the formation of orientation defects that are solvated by adsorbates as well as trajectories calculated on DFT level will be presented.

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2. CP2K, http://cp2k.berlios.de (2000-2004)
3. VandeVondele, J.; Krack M.; Mohamed F.; Parrinello M.; Chassaing T.; Hutter J. Comp. Phys. Comm. 2005, 167, 103.