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COMPETITIVE ADSORPTION OF HNO3 AND HCl ON/IN WATER CLUSTERS AND ICE

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Solvation and ionization of strong acids such as HX (X=Cl, Br), HNO3 etc. have been subjected to many researchers (see for example refs. 1, 2, and references therein). In this study, the competitive adsorption of two strong acids, namely, HCl and HNO3 on/in the water clusters and the surface of crystalline ice slab containing 72 water molecules were investigated at the average temperatures below 140 K. The main tool of this study is on-the-fly molecular dynamics as implemented in the density functional code QUICKSTEP (3) which is part of CP2K package (4). The small water clusters containing both HNO3 and HCl with up to five water molecules were further checked with MP2 level ab initio calculations. The results will be discussed in terms of dynamics, structures, energetics and spectroscopic perspectives.

1. Buch, V.; Sadlej, J.; Aytemiz-Uras, N.; Devlin, J. P., The Journal of Physical Chemistry A 2002, 106, 9374.
2. Escribano, R.; Couceiro, M.; Gómez, P. C.; Carrasco, E.; Moreno, M. A.; Herrero, V. J., The Journal of Physical Chemistry A 2003, 107, 651.
3. CP2K, http://cp2k.berlios.de (2000-2004).
4. VandeVondele, J.; Krack, M.; Mohamed, F.; Parrinello, M.; Chassaing, T.; Hutter, J., Comp. Phys. Comm. 2005, 167, 103.

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