Reaction studies of Al-O clusters in water

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We present several AIMD studies of reactions related on Al-O clusters in water. We have done reaction driven with distance constraint [1,2] and Meta-Dynamics simulations [3]. Of constraint driven reactions we have studied Cl dissociation from Al2O6H8Cl2 [1] and Al2O8H12 + AlO4H6 association reaction. With MetaDynamics we studied Al3OnHm internal reactions. Also a more general discussion of reaction studies using AIMD is given.

[1] J. Saukkoriipi and K. Laasonen, J. Phys. Chem. A. 2008; 112:10873-80.
[2] G.Lanzani et al. to be published
[3] G.Lanzani et al. to be published