Ab initio molecule dynamics simulation of hydroxide reorientation in water

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Reorientation of hydroxide in water

The reorientation time of hydroxide ions in water has recently been experimently studied as a function of temperature from 280K to 324K by Keiding [1] and an activation process below 290K is suggested. A Car-Parrinello Ab initio Molecular Dynamics (AIMD) approach based on Discrete Variable Representation (DVR) basis [2] is used to simulate the microscopic transportation of a hydroxide in 31 water molecules in the same temperature range. The reorientation times obtained from are compared to Keiding's as in Figure 1. The connection between reorientation times and hydroxide hydration shell dynamics, dominant structures, and transport mechanisms as proposed in [3, 4] are further explored, and the possibility of the activation process is discussed.

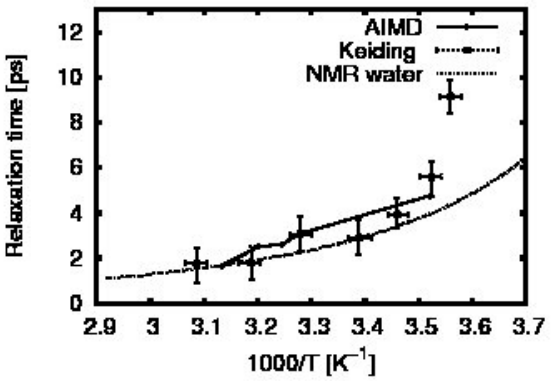

Figure 1: The reorientation times of hydroxide as a function of 1000/T. The linespoints are relaxation time at various temperatures by AIMD. Keiding CCTS experiment data is shown in the figure by the dots with x and y error bars [1]. The dot line is reorientation time of water by NMR[5].

[1] Thogersen *et al*. (2008) *Chem. Phy. Lett*. 009–2614. [2] H.-S. Lee *et al*. (2006) *J. Phys. Chem. A* **110**, 5549. [3] Tuckerman *et al*. (2002) *Nature* **417**, 925. [4] Tuckerman *et al*. (2006) *Acc. Chem. Res*. **39**, 151. [5] Lang *et al*. (1993) *Progr. Nucl. Magnet. Reson. Spectrosc* **25**, 507.

Age, geochemical characteristics of SSZ-type ophiolite in the south Tianshan, China, and subducting direction of the Paleo-Southern Tianshan Ocean

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The LA-ICP-MS (Laser ablation ICP-MS) zircon U-Pb isotopic dating show the formation age of the Kulehu ophiolite, located in Southern Tianshan, Northwestern China, is 418.2±2.6 Ma (MSWD=0.8). It includes two groups of basalts with different geochemical characteristics. The first group with lower $(La/Yb)_N$ (0.35~0.37), high Zr/Nb (39.9~95.1), Ta/Nb (0.07~0.09) and εNd (t) (8.9~12.3), enrichment in LILEs and depletion in HFSEs, especially Nb-Ta negative abnormity suggest that they have the characteristics combining the N-MORB with IAT. Contrastively, the second group with high $(La/Yb)_N$ values (0.96~1.36) and contents of the incompatible elements and Nb-Ta positive abnormity, lower εNd (t) (8.4), Zr/Nb (9.7~10.9) and Ta/Nb values (0.06), are similar to E-MORB.We proposed that Kulehu ophiolite should form in back-arc basin setting on supra-subduction zone (SSZ), and the first group of basalts retaining obvious SSZ signatures are the products of partial melting of depleted mantle in the early stage of back-arc basin resulting from subduction of oceanic slab; as the back-arc system evolves, mantle counterflow provides a relatively fertile mantle upwelling, which resulted in the generation of the second group of basalts. The age of Kulehu back-arc basin ophiolite correspond with that of intra-oceanic island arc volcanic rocks from Bayinbuluke (Ma *et al*. 2008) at the northern margin of Southern Tianshan Orogenic belt, and they constituted the Silurian intra-oceanic arc-basin system in the Paleo-Southern Tianshan Ocean, which also suggest that the subducting direction of Paleo-Southern Tianshan Ocean is not only northward proposed by previous researchers, but also southward.

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[1] Ma Z.P. *et al*. (2008) *Acta Petrologica Sinica* **24**(10), 2289-2300.