## Effect of composition on adsorption of water on perfect olivine surfaces

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The origin of water in the terrestrial planets is controversial. Both comets and asteroids have isotopic properties inconsistent with Earth's water. We are investigating if adsorption of water onto mineral surfaces in the accretion disk could be a viable source of water in the terrestrial planets. Gases coexist with dust in the accretion disk for long periods. The equilibrium H<sub>2</sub>O/H<sub>2</sub> ratio in the accretion disk was ~5x10<sup>-4</sup>, which corresponds to a pH<sub>2</sub>O of ~ 10<sup>-8</sup>bar. Note that the equilibrium partial pressure is probably a lower limit. Astronomical observations show that dust clouds consist of Mg-rich olivine, pyroxenes, and other refractory minerals with radii <1µm. Thus the concomitant presence of water gas and dust with high surface area, points to potential interactions between the two components.

We investigated associative adsorption of a water molecule onto selected olivine surfaces [1], namely the  $\{100\},\{010\}$  and  $\{110\}$ . Surface energy scans on each surface identified both the loci of adsorption and their associated energy. On each surface we identified several high-energy sorption sites (Eads> 100kJ/mole). In environments with low pH<sub>2</sub>O such high-energy sites are most likely the first sites to interact with water molecules. The calculations of [1-2] using pure forsterite suggest that the inner disk could sustain adsorption of water, both associative and dissociative, onto perfect olivine surfaces [3].

To gain a better understanding of the mechanism of adsorption, we are performing minimum energy simulations with olivine with Fa up 14%. We are also conducting molecular dynamic simulations to gain an understanding of the kinetics of desorption. In this talk we will present the results from these latest simulations and quantitatively assess the contribution of this mechanism to the water budgets of the terrestrial planets.

## References

 Stimpfl M., Walker A.M., Drake M.J., de Leeuw N.H. and Deymier P. (2006) *JCG*, in press.
de Leeuw N.H., Stimpfl M., Catlow C.R.A., Drake M.J., Deymier P. and Walker A.M. (2006) *MAPS* submitted.
de Leeuw N.H., Parker S.C., Catlow C.R.A. and Price G.D. (2000) *PCM* 27, 332-341.