WATER IN THE INNER SOLAR SYSTEM: 
INSIGHTS FROM ATOMISTIC AND 
ELECTRONIC-STRUCTURE CALCULATIONS.
Krishna Muralidharan¹, Marilena Stimpfl², Nora H. de 
Leeuw³, Pierre A. Deymier¹, Keith Runge¹ and Michael J. 
Drake²; ¹Material Science and Engineering, University of 
Arizona, Tucson, AZ, 85721, USA, ²Lunar and Planetary 
Laboratory, University of Arizona, Tucson, AZ, 85721, 
USA, ³Department of Chemistry, University College, Lon-
don, 20 Gordon Street, London WC1H 0AJ, UK

Introduction: Water is ubiquitous in the inner solar system, 
but its origins have not been well understood. Suggested sources 
of water include comets, hydrous asteroids, and phyllosilicates 
migrating from the asteroid belt; however, there are problems 
with each of these sources as discussed by Drake [1], who in turn 
proposed that microscopic-level processes such as molecular ad-
sorption occurring during the early stages of planetary formation 
could in fact lead to the delivery of water to the inner solar sys-

tem planets. In order to quantify this possibility, we carried out 
atomistic and electronic-structure calculations examining direct 
adsorption of water on to forsterite grains—the major silicate phase 
in the proto-planetary disk. Specifically, we carried out kinetic 
Monte Carlo (kMC) simulations of water adsorption on various 
surfaces of forsterite based on adsorption energetics obtained 
from atomistic as well as first principles quantum chemical calcu-
lations [2]. The kMC simulations were carried out at thermody-
namic conditions representative of the initial stages of planet ac-
cretion (pressure = 10⁻⁸ bars, temperatures ranging between 700-
1400 K). An equally important issue that was also addressed in 
this work, was the possibility that atomistic-level mechanisms 
could lead to a difference in the D/H ratio of earth-water and ne-

bular-water. Towards this end, we used density functional theory 
(DFT) to calculate the activation barriers for adsorption (via dis-

sociation) and desorption (via recombination) of H₂O and HDO 
molecules on forsterite surfaces in order to see if this could lead 
to preferential retention of HDO.

Results and Discussion: KMC simulations of water adsorp-
tion, show that water could be retained even at conditions corre-
sponding to the accretion disk (high temperatures and very low 
partial pressures), leading to the conclusion that adsorption of 
gaseous water onto dust grains could start from the early stages 
of accretion, and a significant amount of water can be delivered 
to the inner solar system via adsorption. Next, the DFT simula-
tions of H₂O and HDO dissociation showed that the dissociation 
(i.e. adsorption) of H₂O and HDO on forsterite surfaces were 
both exothermic, while the reverse activation barrier (i.e. barrier 
to desorption) for H₂O was around 0.6 KJ/mol (8 % of barrier 
height) lower than that of HDO. Since the desorption rate is re-

lated to the activation energy barrier via a Boltzmann equation, 
the probability of H₂O desorption is incrementally higher, imply-

ing that there could be preferential retention of HDO.

Conclusion: Using atomistic and electronic-structure calcula-
tions, we show that a significant amount of inner solar-system 
planetary water could be delivered via adsorption. Further, using 
density functional theory we show that HDO will be preferen-
tially retained relative to H₂O in adsorption/desorption kinetics. 
Significant work remains to quantify the magnitude of these 
processes, but they must play a role in the origin and isotopic 
composition of Earth’s water.

ran et al., 2008 Icarus 198, 400.