Reaction Pathways through Molecular Dynamics (MD) of Methanol and Hydroxyl cation on Interstellar Water ice surfaces

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July 6th, 2016. Campinas, SP.

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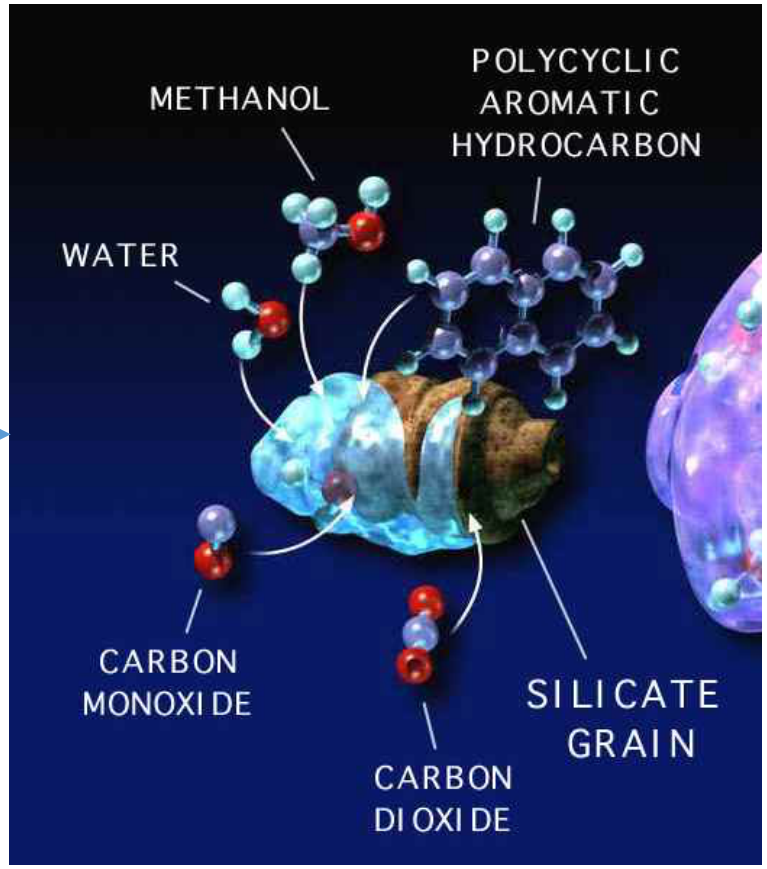
Why Grain-Surface chemistry?



Key Formation Mechanisms

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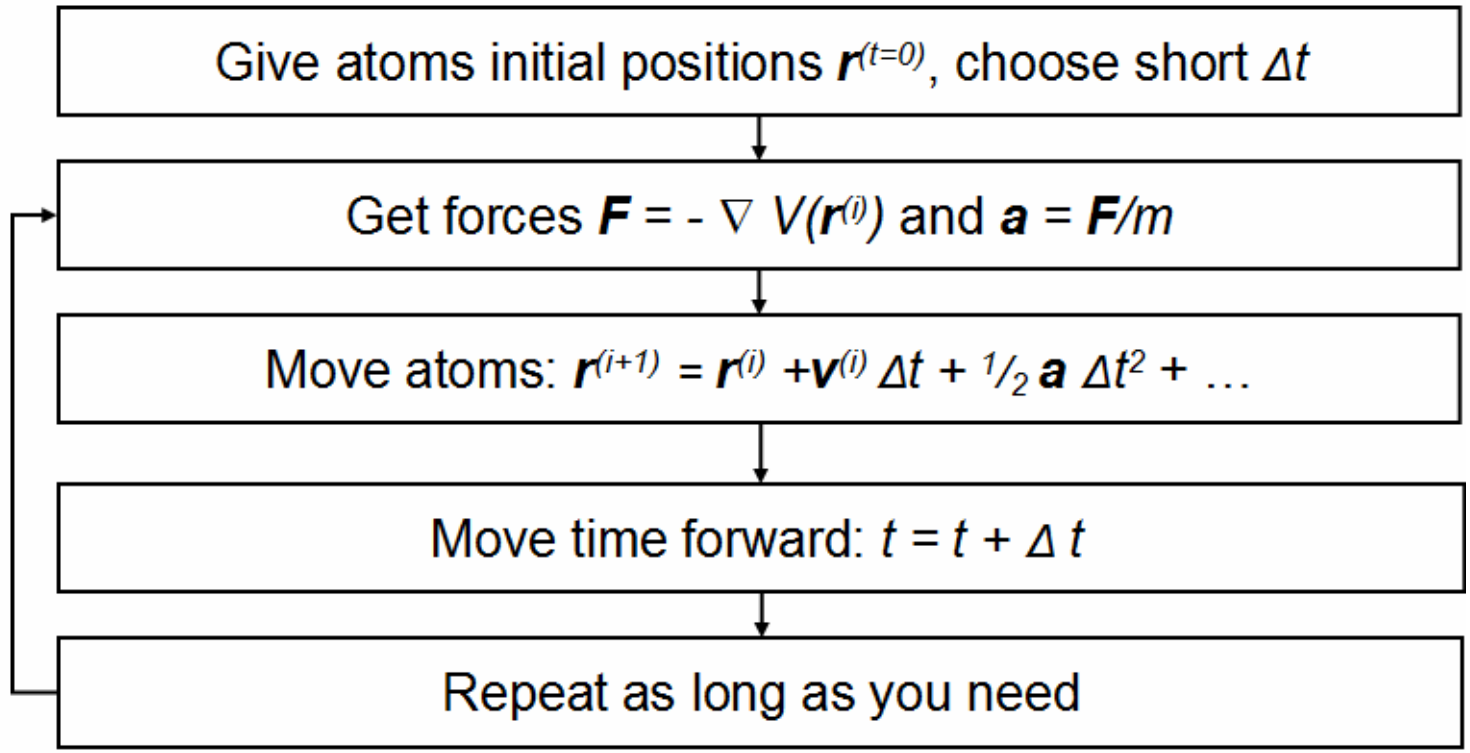
Classical Molecular Dynamics



Since atoms are approximated as discrete particles, interactions of smaller particles cannot be correctly modeled with classical MD.

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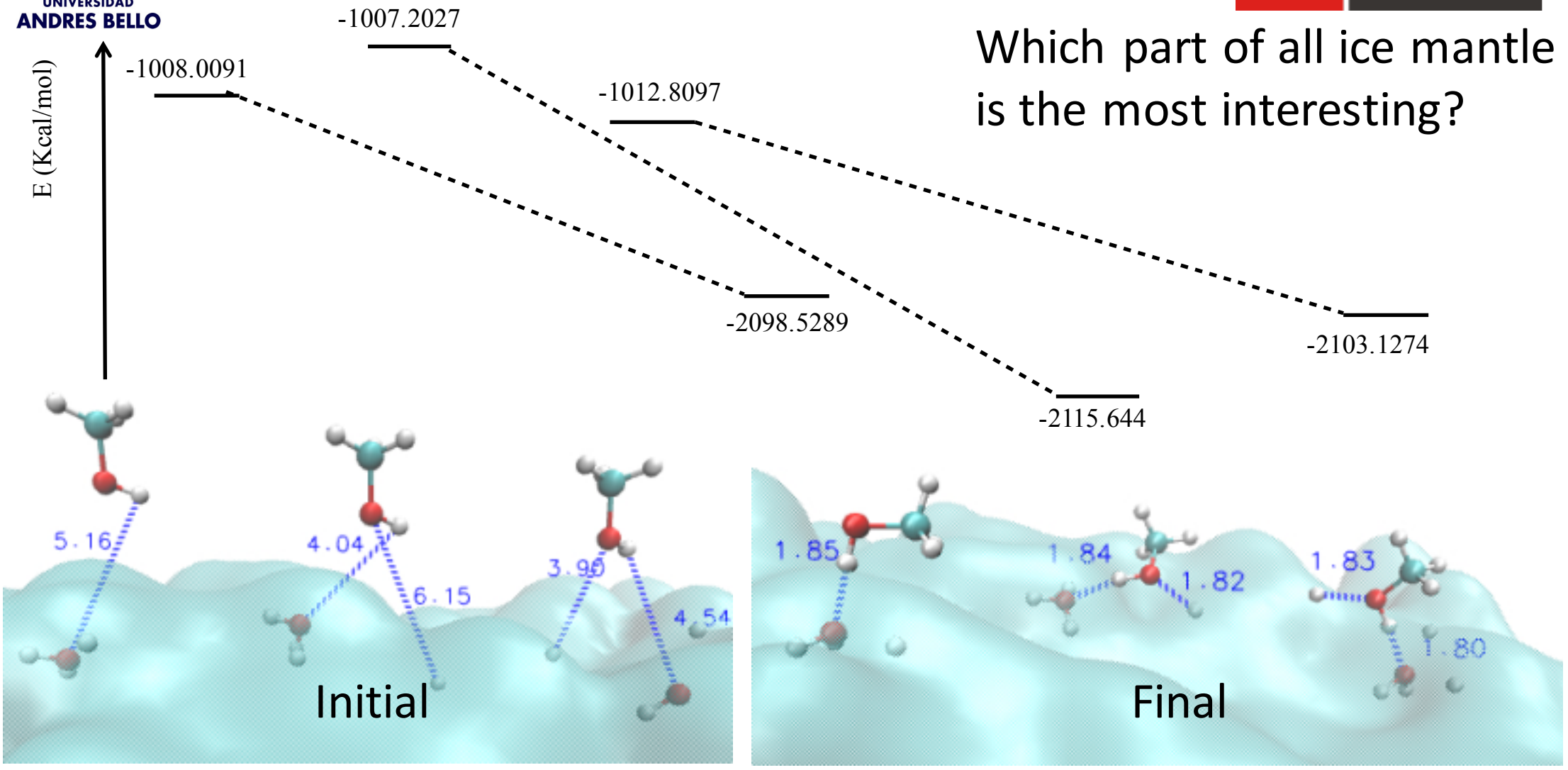
Which part of all ice mantle is the most interesting?



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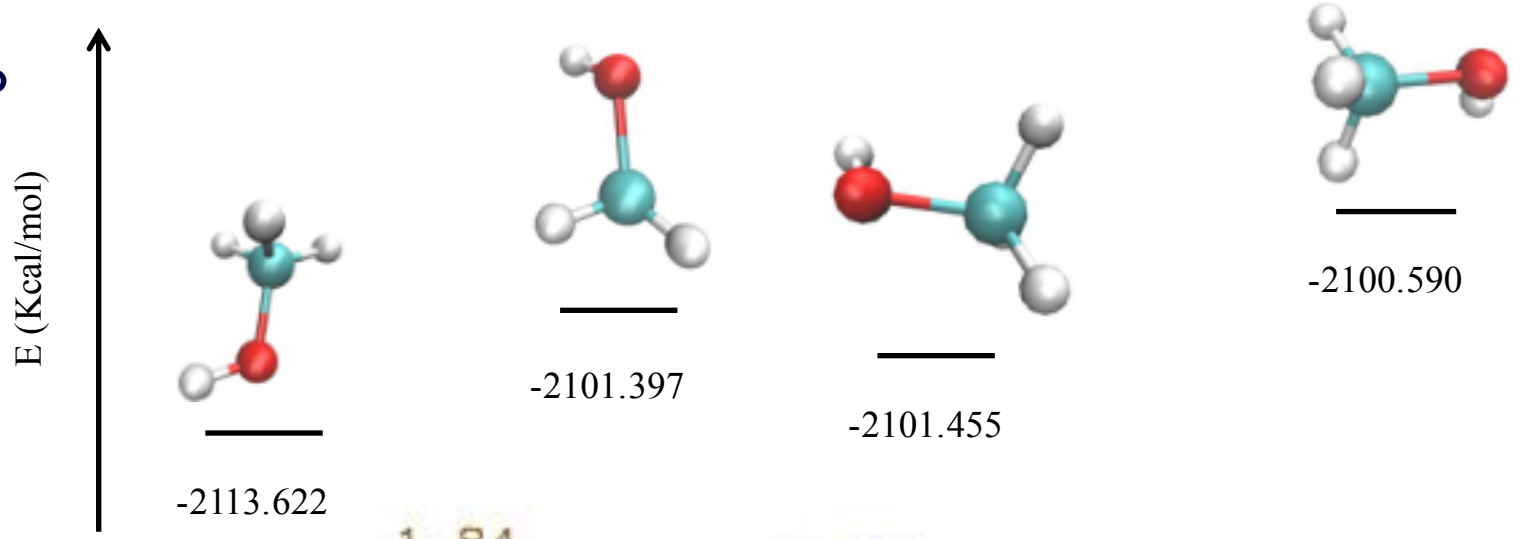

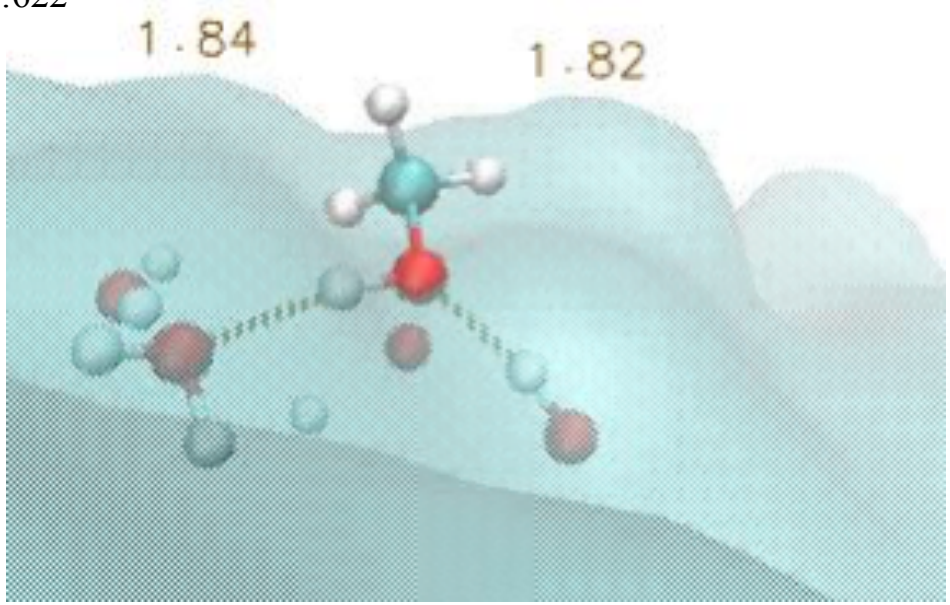

Which the most stable spatial configuration?

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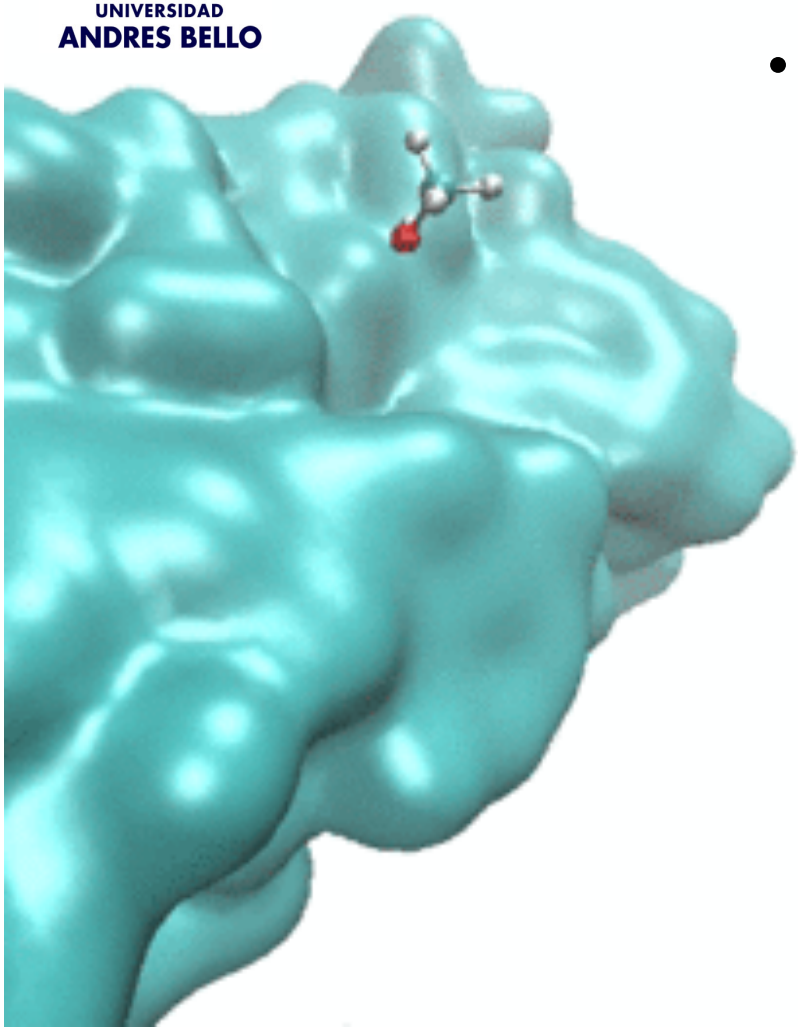
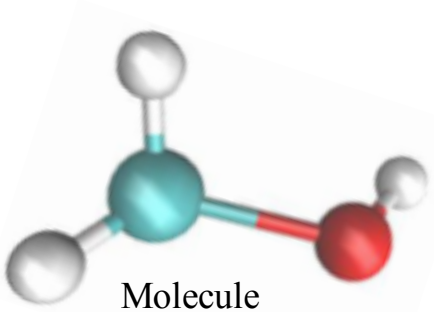
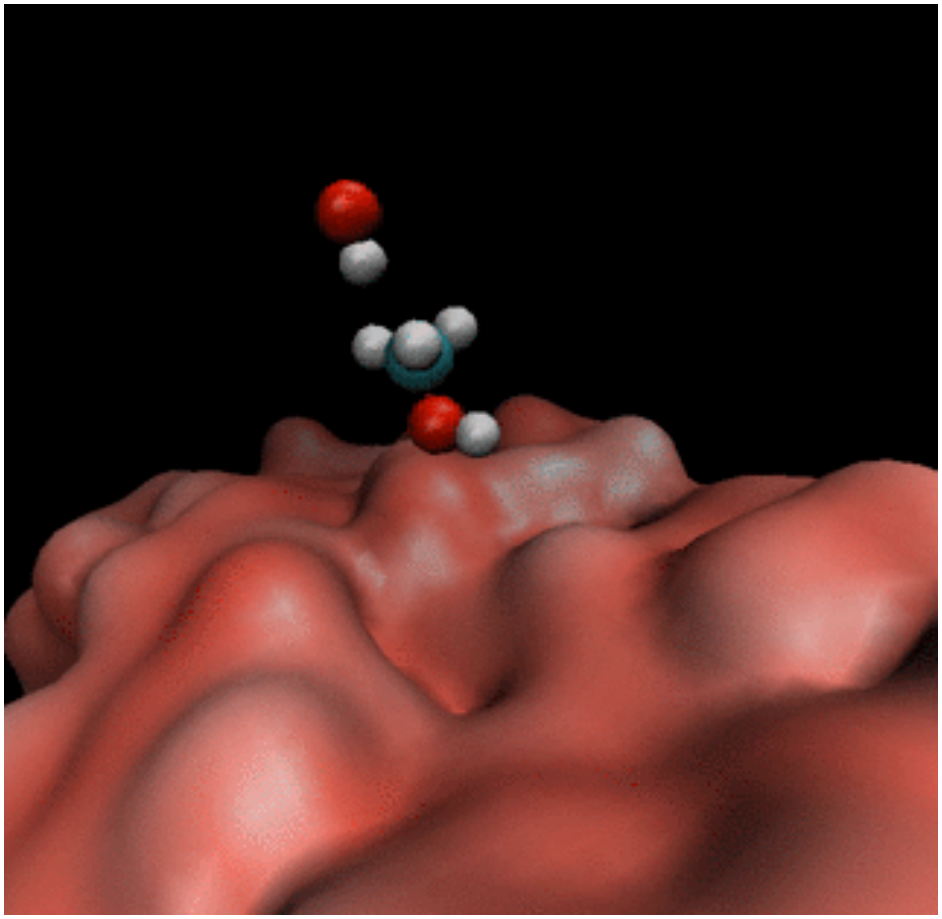


- We found the optimal coordinates configuration as follow:



Molecule

Surface (Ice Mantle)



Why Quantum Molecular Dynamics?

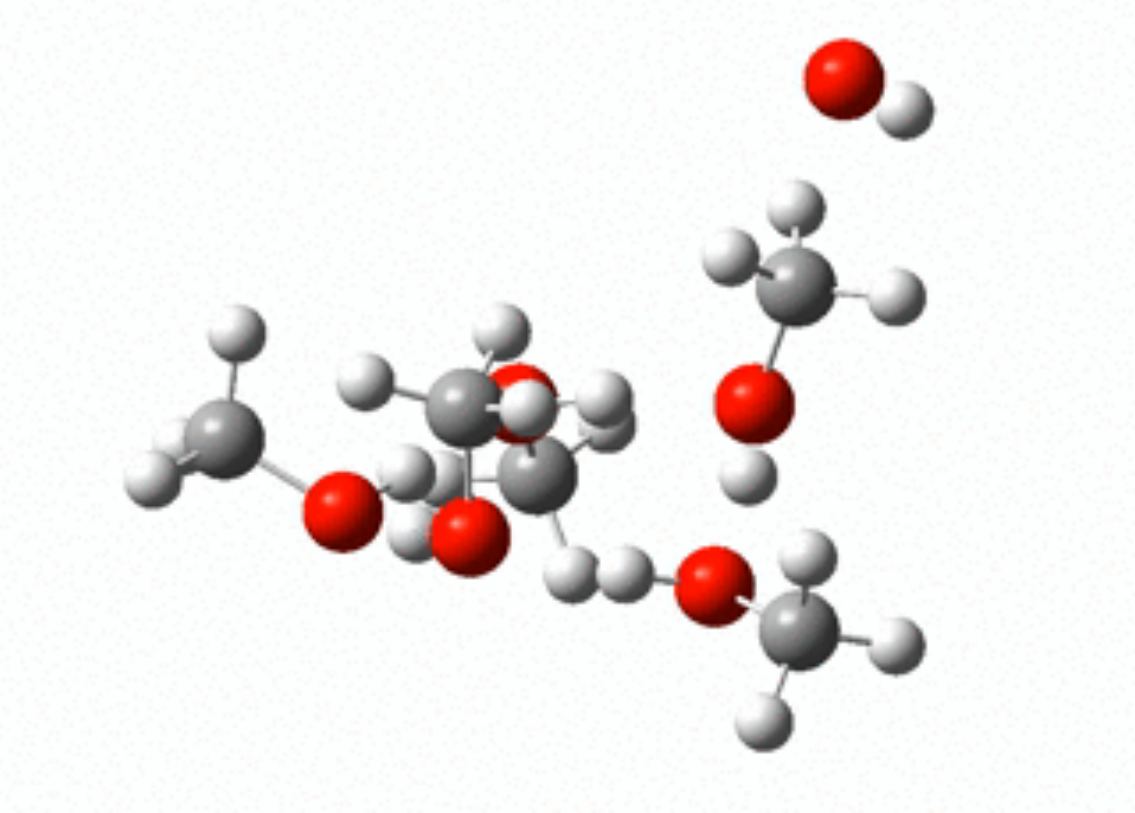
Making and breaking chemical bonds, noncovalent reaction intermediates, and proton or electron tunneling all cannot be simulated with Classical Molecular Dynamics

Quantum Molecular Dynamics

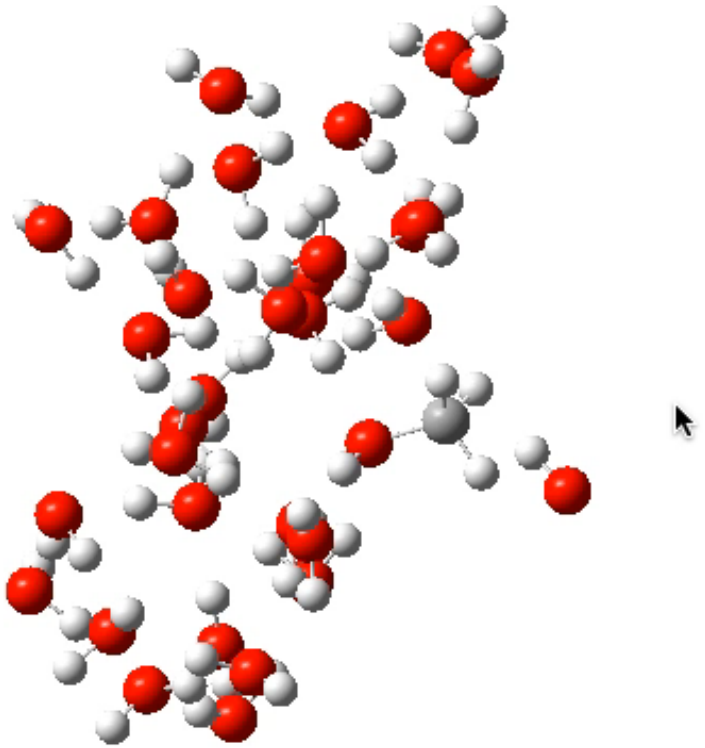
- Quantum molecular dynamics methods exist for simulations that can be more electronically realistic, but at much greater computational cost.

Quantum Molecular Dynamics

- What if we move from gas-phase reaction to grain-surface reaction?



Hover over Ice mantles



Next Theoretical Work

- Scale up to a bigger cluster and use it as a target for the HO^- projectile. A quantum dynamics description.
- Explore as much as we can, different ways to impact the grain surface and describe the chemical reaction on the dust grain.
- Once designed,it is important to use different projectiles to understand different reaction pathways.

Thank You!