Grain surface reaction dynamics from an atomistic perspective

M.A.J. Simons, H.M. Cuppen

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About 60 complex molecules have been observed in space. It is generally accepted that these are formed on the surface of dust grains in cold, dark regions of the Universe. Here the grain acts both as an accretion spot for reactants as well as an energy sink for exothermic reactions. This concept forms the basis for theoretical models that are used in the interpretation of observational data in order to extract molecular details such as reaction mechanisms and surface dynamics.

The exact dynamics of reaction complexes on surfaces are hitherto not considered in the application of such models. Previously, we have raised the question of the limitations on rearrangements of surface reactants and its consequences on possible products [Simons 2020]. Although we showed that the inclusion of non-reactive complexes has but a small effect for single-carbon baring species such as H_2CO and CH_3OH, it stands to reason that this effect will become more significant when larger species (such as glycine) are considered.

Here we have used small molecules as a proxy to study the dynamics of reactants on cold grain surfaces. The results of metadynamics simulations give us the distribution of binding sites and local minima that can provide reaction sites. Using these binding sites we have simulated the meeting of small molecules on a surface. Finally, we used molecular dynamics simulations to provide limits on the rearrangement of reactants in feasible binding sites. Altogether, these simulation results provide a clearer image of how species can meet on cold grain surfaces prior to reaction.

Simons, M. A. J., T. Lamberts, and H. M. Cuppen. "Formation of COMs through CO Hydrogenation on Interstellar Grains." Astronomy & Astrophysics 634 (2020). https://doi.org/10.1051/0004-6361/201936522.