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**Adsorption and reactivity of H atoms towards the Catalytic H2 Formation and Dissociation on Magnesium Silicate Nanoclusters†**

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**Abstract:**

The Universe is rich in molecules and dust particles. While dust particles make up only one mass per cent of the total matter in the interstellar medium (ISM), they play a crucial role in its chemical evolution, by catalysing molecule formation.

Neither radiative association nor ionic processes can account for the observed abundances of H2 in both diffuse and dense clouds. Accordingly, the heterogeneously catalysed association of two H atoms on the surface of dust grains is thought to be the main mechanism for H2 formation in these regions. In oxygen-rich stars the surplus of O atoms can start forming metal oxides in the cooler regions further away from the dying star. The observed stardust silicates are predominantly magnesium-rich pyroxenes (MgnFe(n−1)SiO3), with a significant crystalline fraction (∼10 per cent). While the ISM is refueled with crystalline enstatite and forsterite (MgnFe(2-n)SiO4) grains from the stellar outflows, these must subsequently be efficiently amorphized since in the ISM only amorphous silicates are observed of mainly olivinic composition. A substantial (∼10 per cent) mass fraction of the silicate grain population in the diffuse ISM could be very small (< 15 Å diameter).

We examine in this work a 21 atom forsterite cluster and its possibility to adsorb H atoms with the purpose of understanding the catalysed H2 formation on this model grain. We use the MPWB1K meta-hybrid exchange-correlation functional to compute binding energies with adequate basis sets within the Gaussian 09 code. Global optimisations without any constraint have been carried out in order to get fully relaxed structures, for the bare nanocluster, as well as for when H atoms are adsorbed.

Our work probes the reactivity of ultrasmall silicate dust grain size with respect to H2 formation and dissociation in the gas phase. The results provide a lower size limit benchmark for the astrochemical relevance of such species with respect to that known for the upper size limit of large grains with bulk crystalline facets. Interestingly, our results also provide evidence that ultrasmall non-crystalline nanosilicate dust grains do not simply tend to be more or less effective for H2 formation, but, rather, provide a greater range and variety of chemical pathways for both H2 formation and dissociation. Considering the set of H2 dissociation pathways reported herein together with that reported for the (010) forsterite surface (Goumans et al. 2009), we find that in all cases Ebind(of 2 chemisorbed H) has a strong linear relation to the H2 dissociative barrier height.

† Kerkeni B & Bromley ST (*MNRAS)* 2013.

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Contribution: Oral  Poster