

## Molecular hydrogen formation on the surface of cosmic dust and the infrared emission as an astronomical new probe

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In interstellar space, molecular hydrogen ought to be formed on the surface of cosmic dust grains. Molecular dynamics computer simulations were performed to investigate the whole fundamental processes of H<sub>2</sub> formation on the amorphous water ice as a model surface of icy mantles of dust grains. It was found that H<sub>2</sub> newly formed on the dust surface should be in highly vibrationally and rotationally excited states in the ground electronic state via the formation pumping mechanism. The infrared H<sub>2</sub> emission spectrum arising from formation pumping was calculated. It was found that it can be an astronomical new probe.

In interstellar space, molecular hydrogen ought to be formed on the surface of cosmic dust grains. Molecular dynamics (MD) computer simulations were performed to investigate the H<sub>2</sub> formation reaction on the amorphous water ice as a model surface of icy mantles of dust grains. The following fundamental processes of H<sub>2</sub> formation on dust surfaces were examined: 1) sticking process of incident H atoms onto the dust surface, 2) diffusion process of H atoms on the dust surface, 3) reaction process of two H atoms on the dust surface, and 4) ejection process of the product H<sub>2</sub> molecule from the dust surface back into gas phase. The product energy distribution was also examined.

It was found that H<sub>2</sub> newly formed on the surface of dust grains should be in highly vibrationally and rotationally excited states in the ground electronic state via the formation pumping mechanism. The infrared H<sub>2</sub> emission spectrum dominated by formation pumping was calculated. It was found that the resulting spectrum should be detectable in interstellar space, and that it can be discriminated from that dominated by UV pumping as well as has information about the property of dust. The infrared H<sub>2</sub> emission arising from formation pumping can be an astronomical new probe.