Adsorption Energies of Atoms and Molecules on Amorphous Ice Surface: A Systematic Estimation Based on Quantum Chemistry Calculation

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Chemical evolution from atoms to interstellar molecules is a key to explore the origin of molecules. However, collision of two or more atoms in the vacuum is elastic because an excess energy from formation of a molecule is not dissipated to the vacuum. Therefore, chemical reactions on the inter-stellar dust play a key role to form various molecules in the interstellar medium. The first step of such chemical reactions is adsorption of atoms onto the dust surface. In dense molecular clouds, the interstellar dust is generally covered by amorphous ice which mainly consists of water molecules. Thus, the adsorption onto amorphous ice surface at the low-temperature is of considerable importance to explore the chemical evolution in this stage.

In this work, we proposed a new computational model to systematically estimate adsorption energies of atoms and molecules onto the low-temperature amorphos ice surface based on quantum chemistry calculations, as following: (1) Clasical MD annealing from 300K to 10K to sample small amorphous water clusters (including 20 water molecules), (2) add an atom randomly surrounding the water cluester and optimized geometry based on quantum chemistry calculation (density functional theory with ω-B97XD functional), (3) search the maximum adsorption energy for each water cluster, and (4) average the maximum adsorption energies over the cluster samples.

Taking the maximum adsorption energy incorporates local geometry relaxation during long time-scale fructuation, and averaging over them averages stable adsorption site in the amorphous water ice surface.

Table. Calculated adsorption energies

	$C(^3P)$	$N(^4S)$	$O(^3P)$
$E_{ads.}$	14,100	400	1440
Std. Error	420	30	160
Exptl.	N/A	720	1410

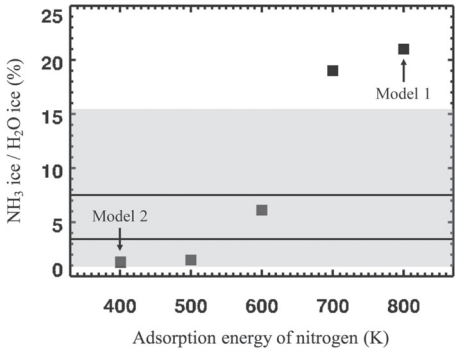

Figure. NH_3 abundance estimated by using various adsorption energies of N.

The adsorption energies of C, N, and O atoms were estimated to be 14,100 K, 400 K, and 1440 K, respectively (see Table). Those of N and O are well consistent with the laboratory experiments by Minissale.[1] Interestingly, the adsorption energy of C atom was estimated to be considerably large, clearly indicating that the adsorption of C atom is clarified by chemisorption. On the other hand, the calculated adsorption energy of N atom was slightly lower than the experimental value. As a result, diffusion process is enhanced even at the low-temperature amorphous ice surface, and therefore, chemical abundance of N_2 increases while that of NH_3 decreases (see Model 2 in the Figure). Consequently, our newly proposed scheme to estimate the adsorption energy will give a new insights into the chemical evolution at the low-temperature interstellar space.[2]

Reference:

[1] Minissale, M., Congiu, E., & Dulieu, F. 2016, A&A, **585**, A146.
[2] Shiminishi, T., Nakatani, N., Furuya, K., & Hama, T. 2018 APJ, **855**, 27.