Theoretical Investigations on Fundamental Properties of All-Nitrogen Materials: Ⅰ. Prediction of Crystal Densities

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Abstract: In order to predict the crystal density of all-nitrogen materials accurately, the 'specific' molecular force field of all-nitrogen materials was established based on the quantum chemistry calculation method. The crystal densities of twenty kinds of all-nitrogen molecules were calculated by predicting the crystal packing structure. Results show that the crystal densities for five kinds of all-nitrogen molecules with cage type including $N_4(T_d)$, $N_6(D_{3h})$, $N_8(O_h)$, $N_{10}(D_{5h})$, and $N_{12}(D_{6h})$ are 1.81, 2.08, 2.47, 2.46 g·cm^{-3} and 2.57 g·cm^{-3}, respectively. As the number of nitrogen atoms increases, the change in crystal densities of all-nitrogen molecules with cage type is different from the progressive trend in literatures, but at $N_8(O_h)$, there is a mutation, which reflects the specific force field parameters.

Key words: force field parameter; quantum chemistry; cage type structure; binding energy

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