

Vacancy Bjerrum Defects in s-II type Clathrate Hydrates*

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Clathrate hydrates are crystalline, cage-like structures formed by hydrogen-bonded water molecules that encapsulate guest gas molecules. The hydrate structure that forms depends strongly on the size of the guest species and its chemical interactions with water or ice¹. One of the most common and widely studied hydrate phases is structure II (sII). In this work, we present a density functional theory (DFT) investigation of vacancy–Bjerrum defect complexes in sII hydrates, focusing on their structure, energetics, and dynamics. These defects are believed to play a crucial role in hydrate formation processes and in facilitating the transport of guest gas molecules through the water cages^{2–4}.

References:

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