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Interaction of Water Layers on Calcite Surfaces[1]
RASHID HAMDAN, HAI-PING CHENG, University of Florida — Calcite is a mineral of great interest because its abundance in both geological and biological systems. While the $\{10\hat{1}4\}$ surface largely dominates the calcite morphology, other surfaces consisting of $\{10\hat{1}4\}$ terraces and steps are important for the crystal dissolution or growth in aquas environment. We use ab-initio calculations to study the interaction of single water molecule and one and two water layers with the flat $\{10\hat{1}4\}$ calcite surface and two step surfaces: $\{10\hat{1}3\}$ and $\{10\hat{1}5\}$ made of $\{10\hat{1}4\}$ terraces offset by one atomic layer along the $\{10\hat{1}1\}$ and the $\{0001\}$ surface respectively. Preliminary results show that the first layer of water bond strongly to the calcite surface. However, dissociation of the water molecules is not favored on the surface.

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