Interaction of Water Layers on Calcite Surfaces

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\bar{1}4\} surface largely dominates the calcite morphology, other surfaces consisting of \{10\bar{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\bar{1}4\} calcite surface and two step surfaces: \{10\bar{1}3\} and \{10\bar{1}5\} made of \{10\bar{1}4\} terraces offset by one atomic layer along the \{10\bar{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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Rashid Hamdan
University of Florida

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