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Interaction of diamond (1x1) and (2x1) reconstructed (111) surfaces with oxygen: A density functional theory study (DFT)

The properties of oxygen atoms on C(111)-(1x1) and the (2x1) reconstructed surfaces have been investigated using DFT. The on-top site is preferred by oxygen atoms on the (1x1) surface, while the bridge site is favourable on the (2x1) reconstructed surface. Other properties like stability and workfunction are also reported.

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