Two-Dimensional Portlandite: From Bulk to Single Layer

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$Ca(OH)_2$ crystals, well-known as Portlandite, are grown in layered form and we found that they can be exfoliated on different substrates. We performed first principle calculations to investigate the structural, electronic, vibrational and mechanical properties of bulk, bilayer and monolayer structures of this material. Different from other lamellar structures such as graphite and transition metal dichalcogenides, intralayer bonding in $Ca(OH)_2$ is mainly ionic, while the interlayer interaction remains a weak dispersion-type force. Unlike well-known transition metal dichalcogenides that exhibit an indirect-to-direct band gap crossover when going from bulk to a single layer, $Ca(OH)_2$ is a direct band gap semiconductor independent of the number layers. The in-plane Young's modulus and the in-plane shear modulus are predicted to be quite low while the in-plane Poisson's ratio is larger in comparison to the one in graphene. We measured the Raman spectrum of bulk $Ca(OH)_2$, and identified a low frequency mode E_u (T) at 280 cm^{-1} and a high frequency -OH stretching mode A_{1g} at 3620 cm^{-1} . In this study bilayer and single layer Portlandite ($Ca(OH)_2$) are predicted to be stable and their characteristics are analyzed in details. Our results can guide further research on ultra-thin hydroxides.

References

[1] E. Arkin et al. submitted to Phys Rev B (2014)

Figures