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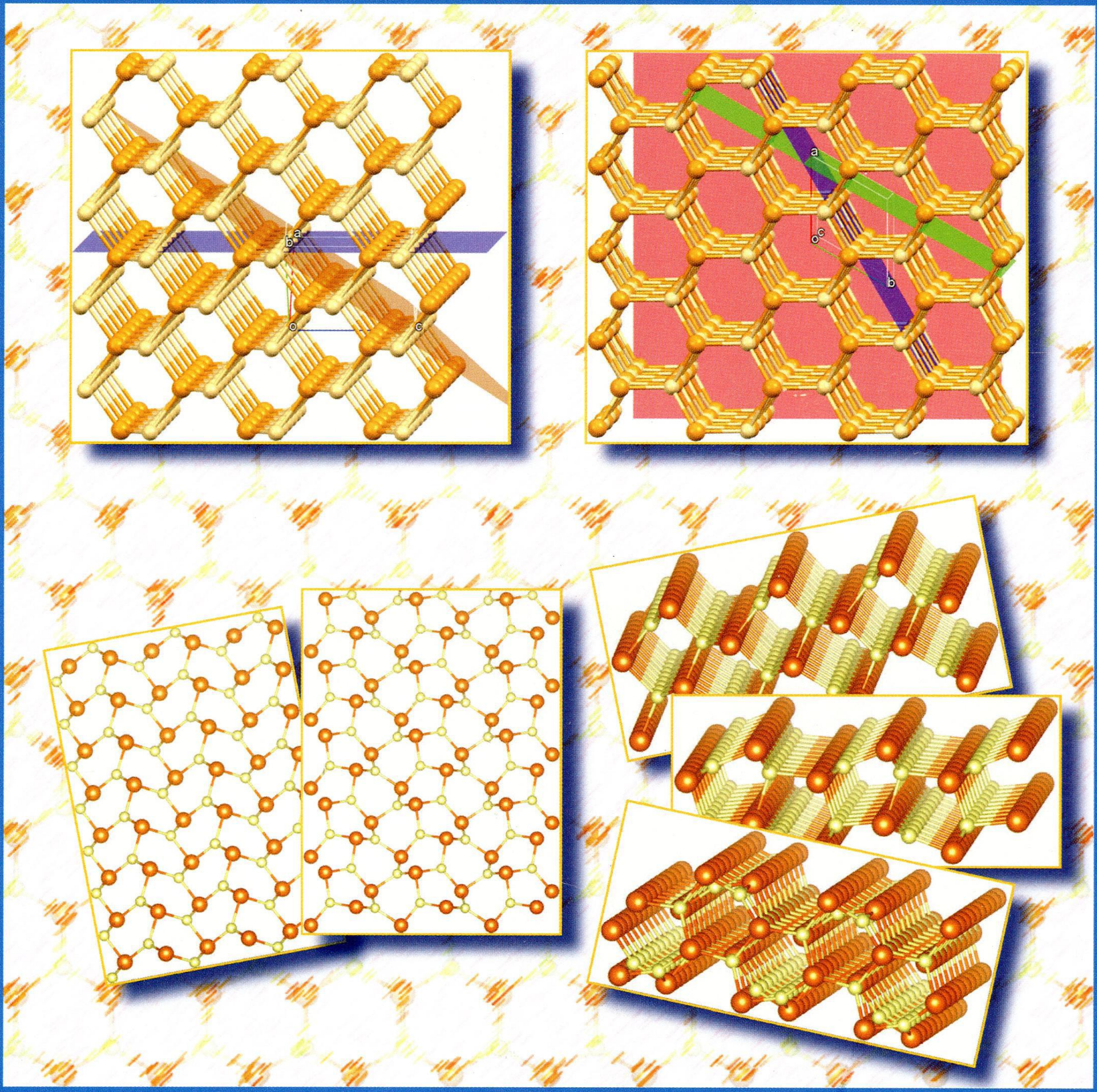

Freestanding Honeycomb Sheets of II–VI Cadmium Chalcogenides (see page 16236)

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ON THE COVER: Freestanding honeycomb sheets of II–VI cadmium chalcogenides. Two-dimensional (2D) nanocrystals of CdX (X = S, Se, Te) typically grown by colloidal synthesis are coated with organic ligands (or surfactants). In light of the fact that various 2D lamellar inorganic–organic hybrid structures $[Cd_nX_n(L)_m]$ (where X = S, Se, or Te; L = alkylamine ligand; $n = 1-3$; and $m = 0.5$ or 1 depending on L) have been made experimentally, we envision that the novel, freestanding 2D layered sheets of CdX will be made soon by exfoliating lamellar hybrid intermediates followed by removing the alkylamine ligands with heating. In this study, we present comprehensive and systematic theoretical predictions of the geometric structures, energetics, and electronic properties of freestanding 2D layered sheets of CdX, all possessing pseudo honeycomb lattices. Surprisingly, given the same geometrical connectivity, these 2D honeycomb sheets adopt various surface corrugations, which are accompanied by different energies and electronic properties. These newly predicted 2D layered materials provide tunable and diverse band gaps, complementary to their bulk phases, and thus offer a novel set of 2D layered materials valuable for a wealth of applications such as photovoltaic and solar water splitting. See page 16236.

Articles

Energy Conversion and Storage; Energy and Charge Transport

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Plasmonics, Optical Materials, and Hard Matter

Physical Processes in Nanomaterials and Nanostructures

Additions and Corrections

Ⓢ Supporting Information available via online article