Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information //Two-Dimensional Buckled Tetragonal cadmium chalcogenides, including CdS, CdSe, and CdTe Monolayers as Photo-catalysts for Water Splitting

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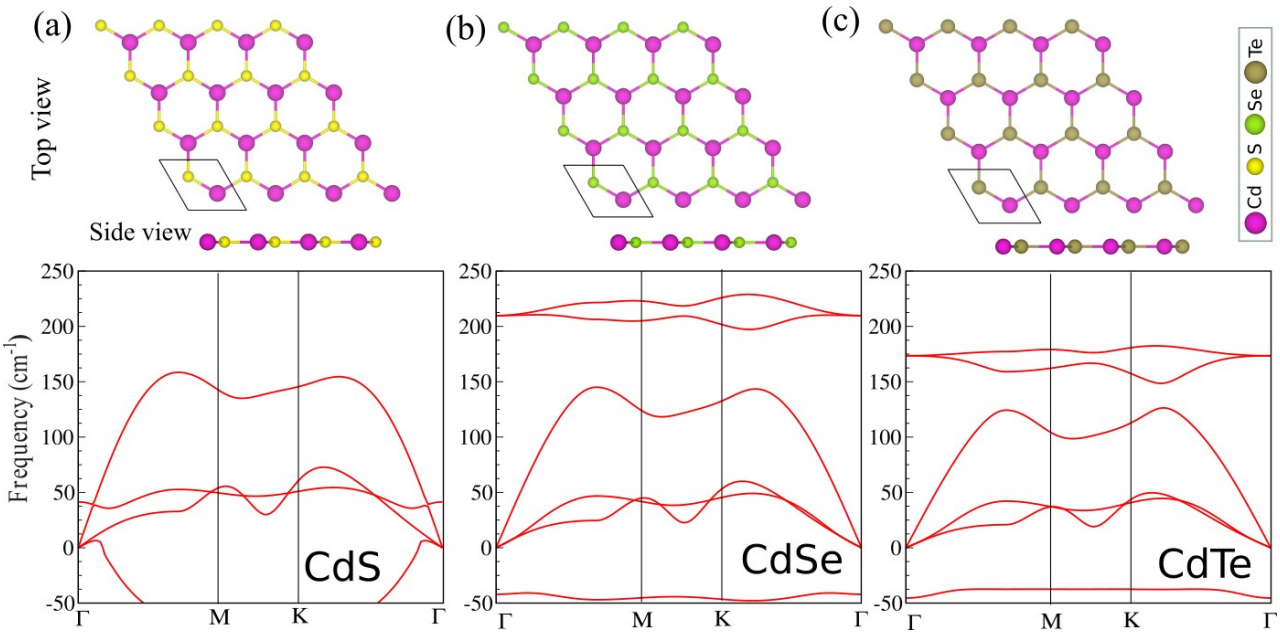

Fig. S1 Atomic structures (top) and phonon band dispersion (bottom) of (a) CdS, (b) CdSe and (c) CdTe monolayers.

In the hexagonal phase which was previously reported by Jiajun Wang [1]et.al, As it is seen in the figure, negative phonon modes are appearing in the hexagonal phase of the 2D CdS, CdSe and CdTe monolayer structures showing their kinetically instabilities.

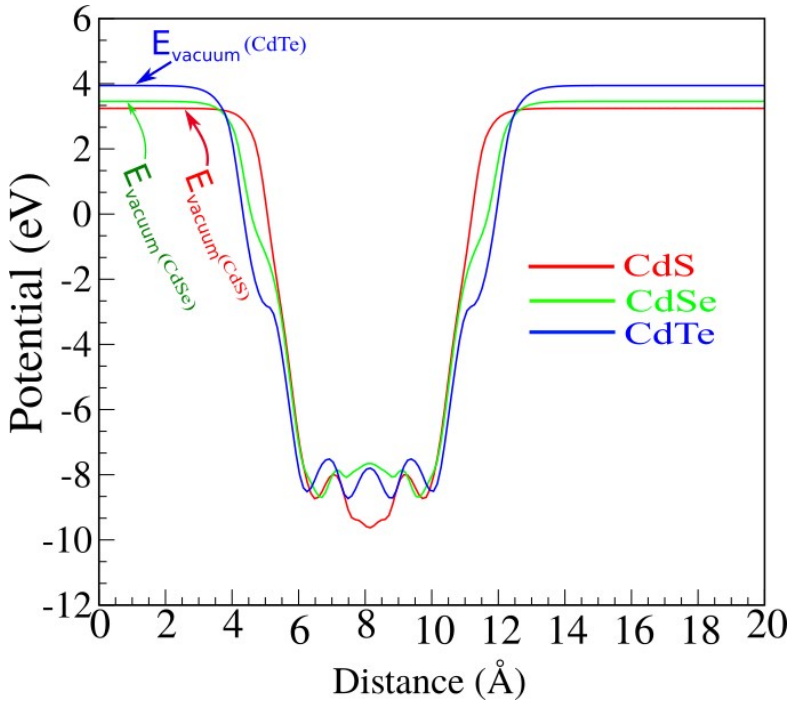

Fig. S2 Electrostatic potential for the CdS, CdSe and CdTe single layers.

[1] Single-layer cadmium chalcogenides: promising visible-light driven photocatalysts for water splitting, Phys. Chem. Chem. Phys., 2016, 18, 17029.