Electronic Supplementary Material (ESI) for New Journal of Chemistry.
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Supplementary information// Novel two-dimensional ZnO_2 , CdO_2 and HgO_2 monolayers: a first-principles-based prediction

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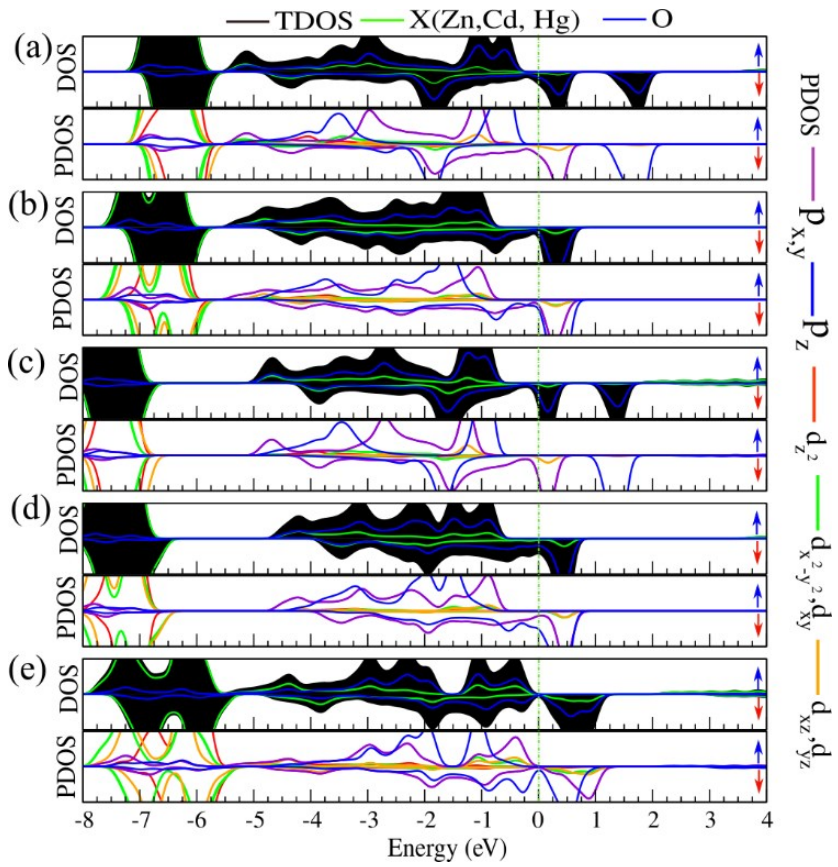

Fig. S1. The contribution of different atomic orbitals for (a) ZnO2-1H, (b) ZnO2-1T, (c) CdO2-1H, (d) CdO2-1T and (e) HgO2-1T.

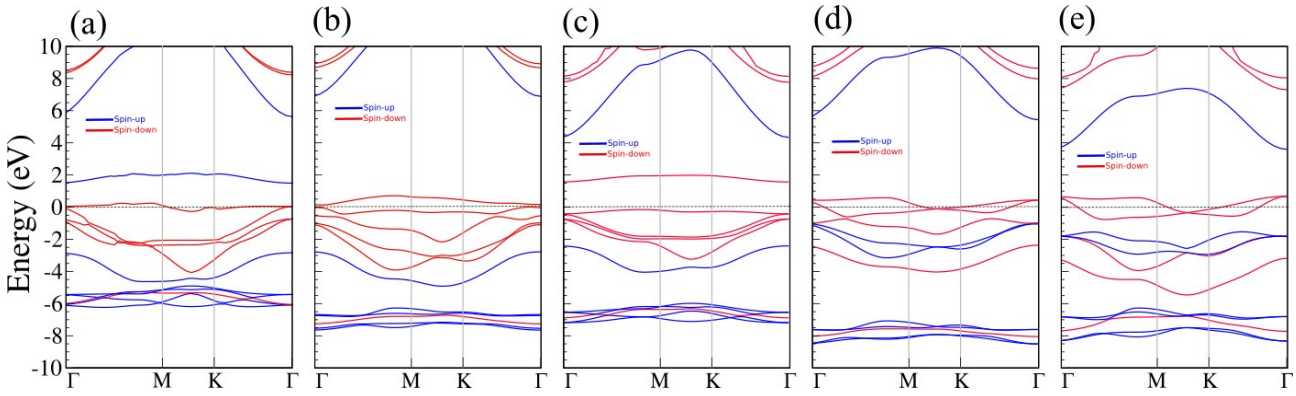

Figure S2. Electronic band structure of (a) ZnO 2 -1H, (b) ZnO 2 -1T, (c) CdO 2 -1H, (d) CdO 2 -1T and (e) HgO 2 -1T monolayers within HSE06 functional. The zero of energy is set to Fermi-level.

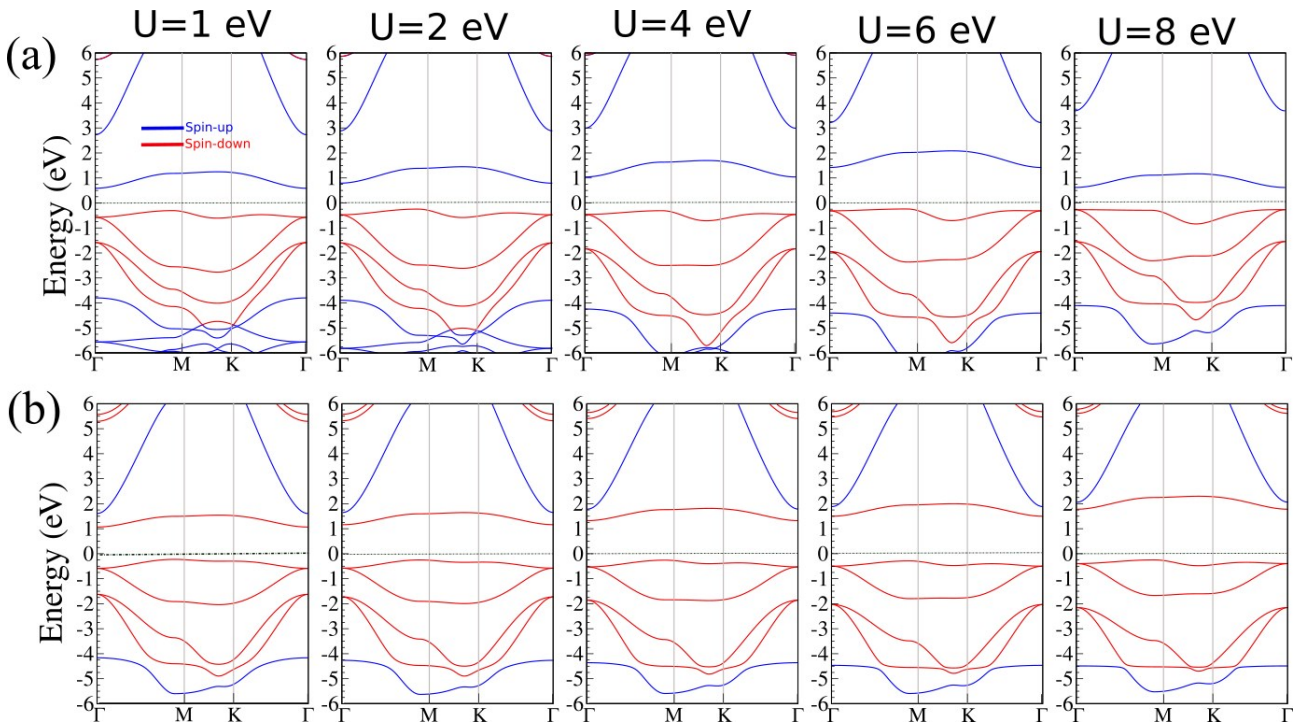

Figure S3: (a) Electronic band structure as a fucnction of Hubbard U for the (a) ZnO 2 -1H and (b) CdO 2 -1H monolayers. The zero of energy is set to Fermi-level.