Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information// Investigation of doping and strain on the electronic properties of single layers of C6N6 and C6N8 : A first principles study

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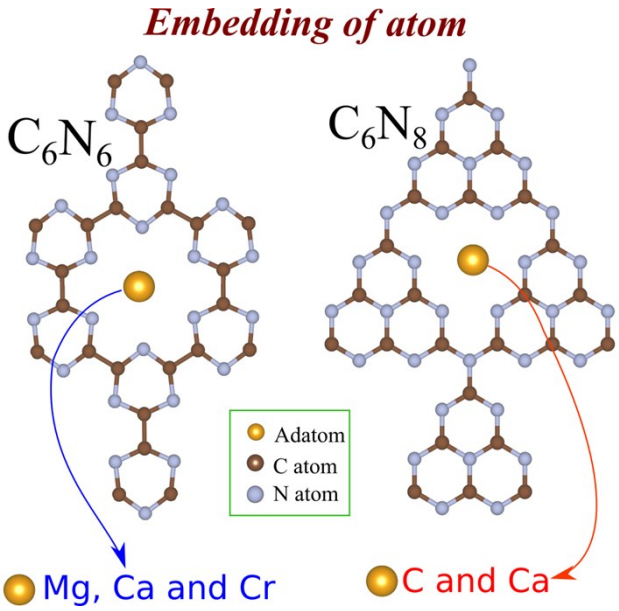

Fig. S1: : Schematic atomic structure for embedded atoms into C6N6 (left) and C6N8 (right).

A schematic view of the embedded atom into holey site of C6N6 and C6N8 monolayers are shown in Fig. S1. For the different atoms considered in our present study, the stable binding sites are uniformly at the nanopore.

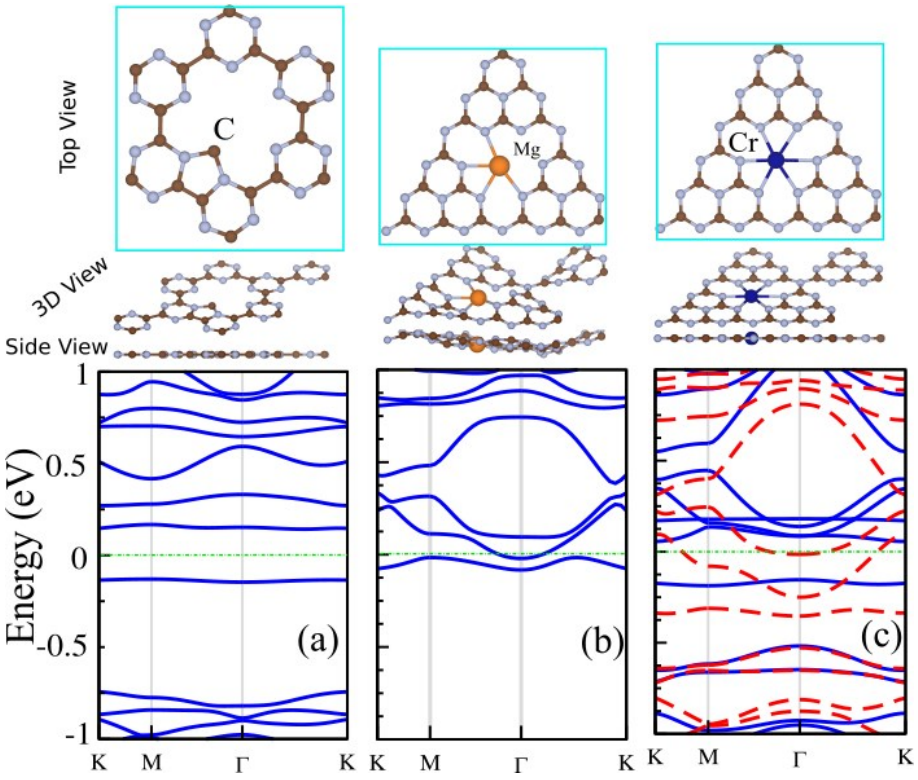

Fig. S2. Electronic structure of (a) C@C6N6 , (b) Mg@C6N8 and (e) Cr@C6N8. The zero of energy is set at Fermi-level. Top, 3D and side views of optimized structures of studied systems are shown in top of panel. The zero energy is set to the Fermi-level.

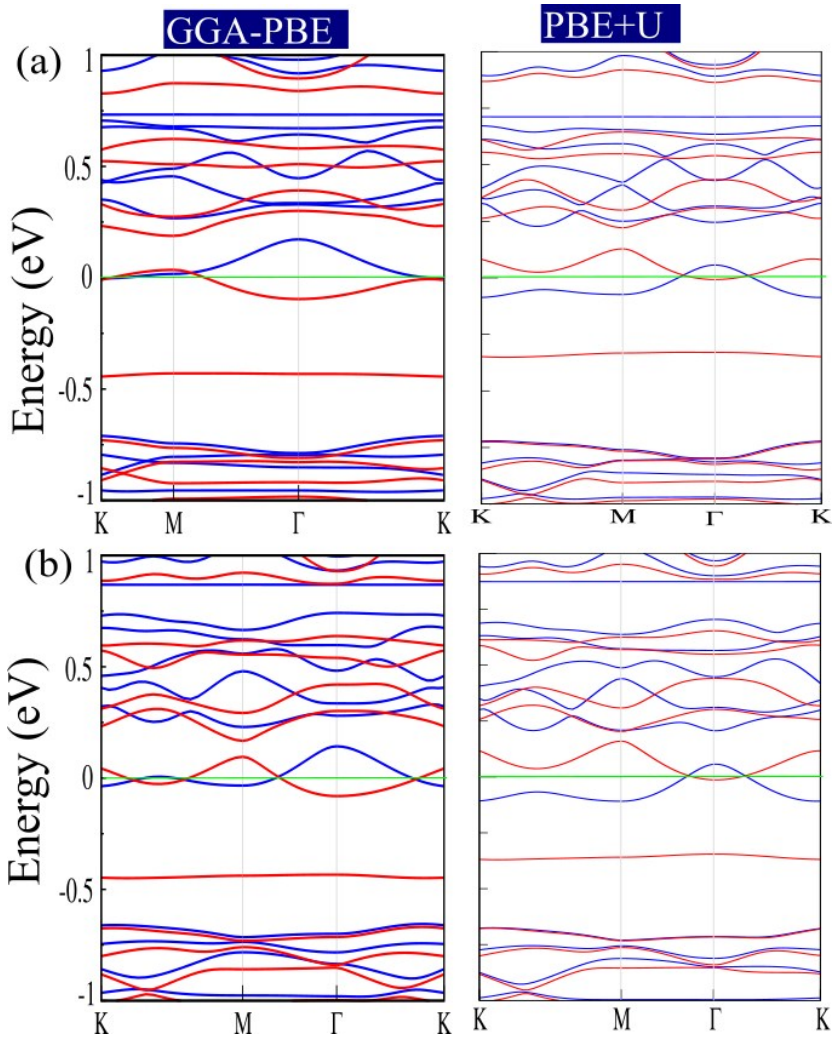

Fig. S3: Electronic structure of (a) Cr@ C6N6 , without and with considering of Hubbard U effect. (b) Cr@ C6N6 upon -2% strain, without and with U effect. The zero energy is set to the Fermi-level.

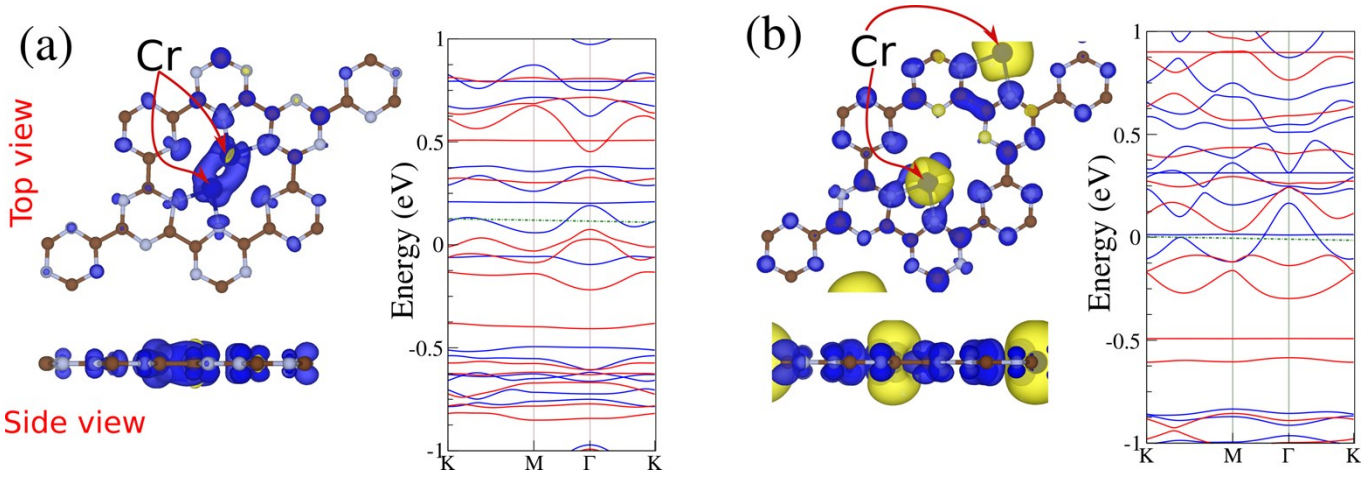

Fig. S4. Differences spin density of Cr embedded in (a) one and (b) two neighboring cavities of C_6N_6, positive and negative are represented by blue and yellow, respectively. Electronic band structure indicated in the left pannel.