

Figure S1. The atomic structure of graphene with substitutional graphitic oxygen (G^*). The oxygen is located in one plain with graphene carcass. There are two C-O bond lengths of 1.47 Å (blue line), and one C-O bond length of 1.48 Å. (green line). The C-C bond length near O atoms decreases to 1.40 Å (orange).

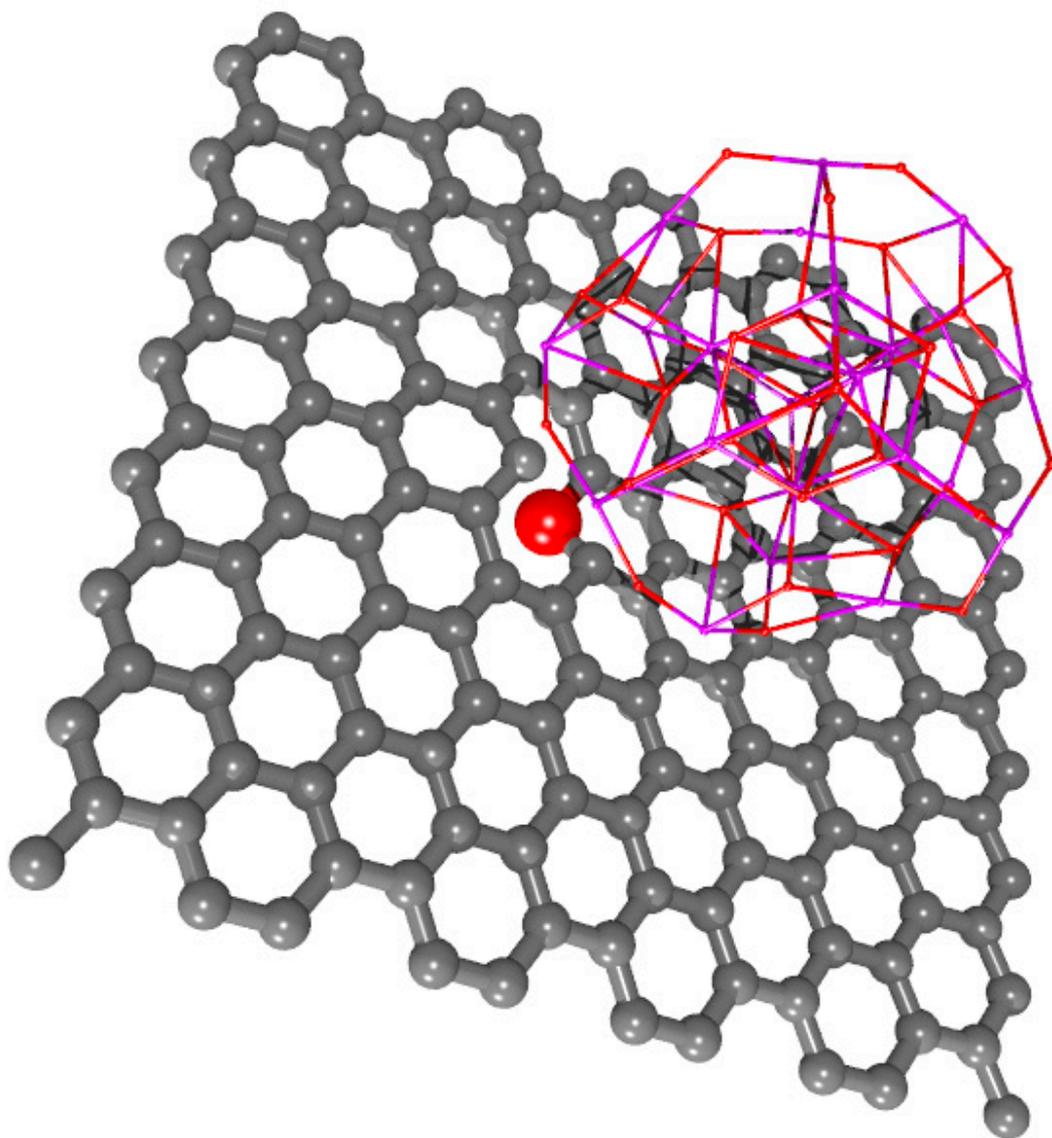


Figure S2. The atomic structure of graphene with substitutive graphitic oxygen after attachment Co_3O_4 nanocube. It's seen that one of C–O bonds was broken.

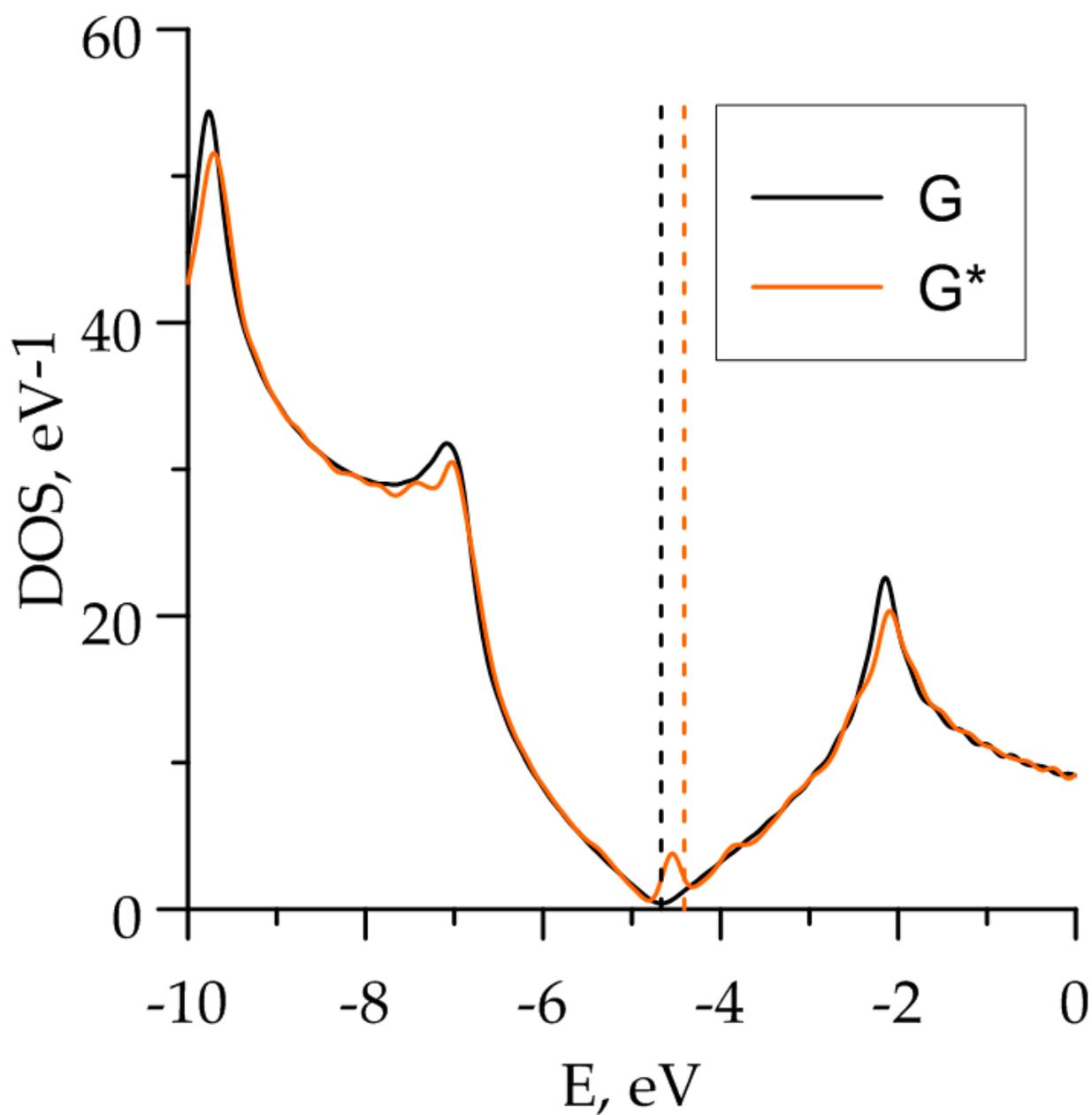


Figure S3. The density of state (DOS) for pure graphene (G) and graphene with substitutional graphitic oxygen (G*). Dashed lines mark Fermi-level.

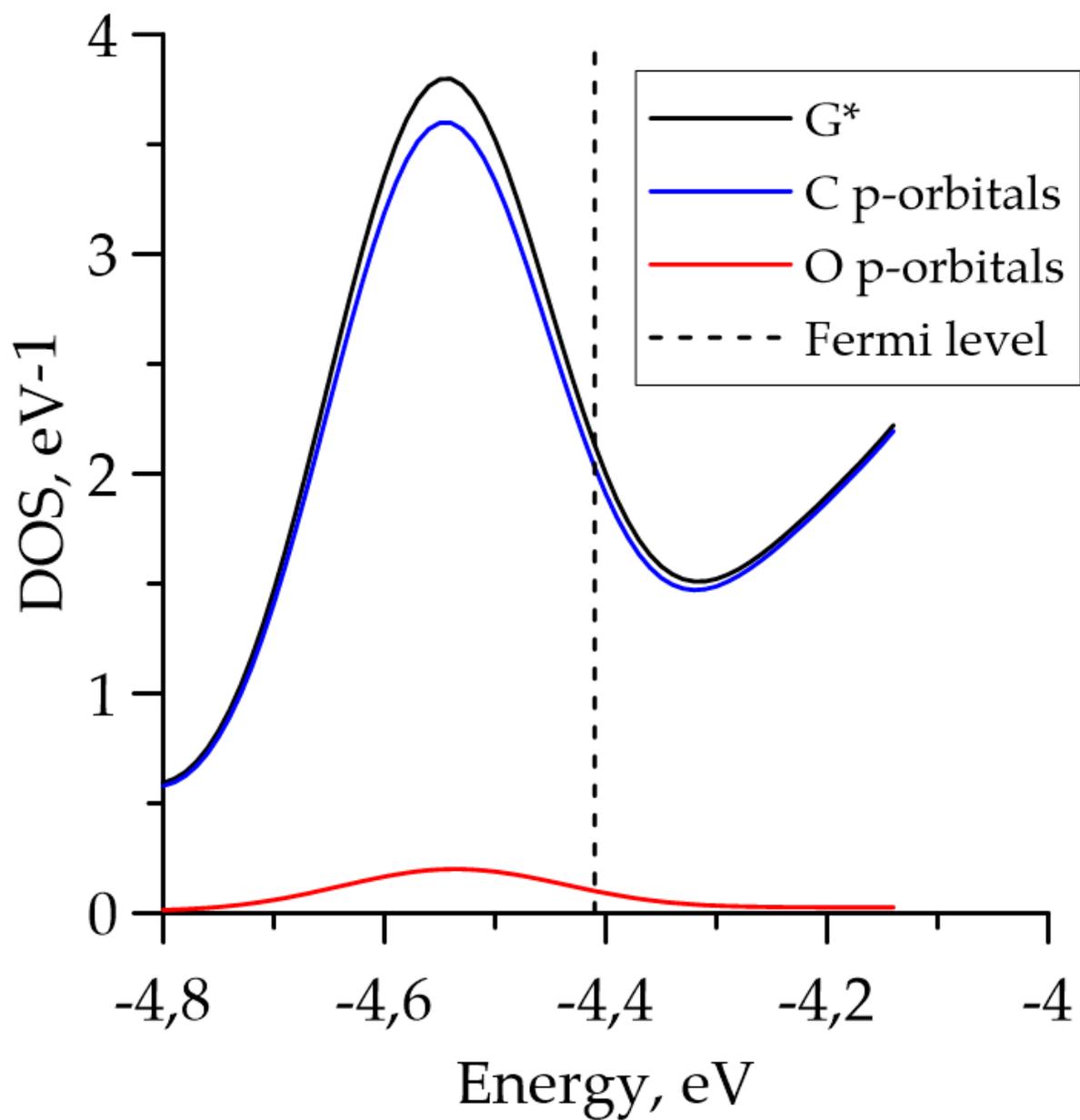


Figure S4. The total density of state (DOS) for graphene with substitutional graphitic oxygen (G*) and partial DOS (pDOS) for p-orbitals of carbon and oxygen atoms. Dashed line marks Fermi-level.