Supplementary Information

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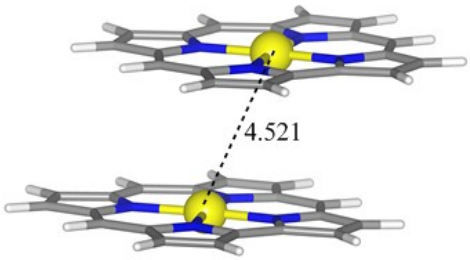

Figure S1. Optimized structures of **Au_2(Au-cor)$_2$**.

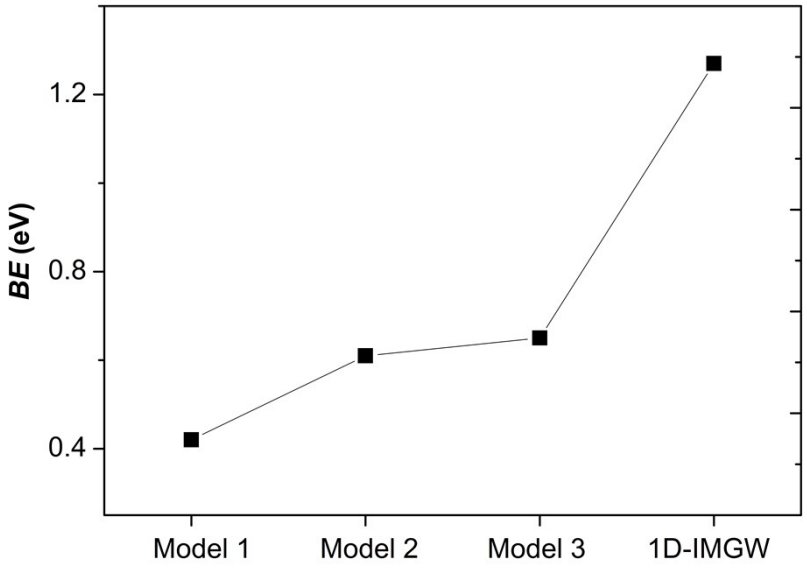

Figure S2. Binding energies (*BE*) four **Model 1**, **Model 2**, **Model 3** and 1D-1MGW.

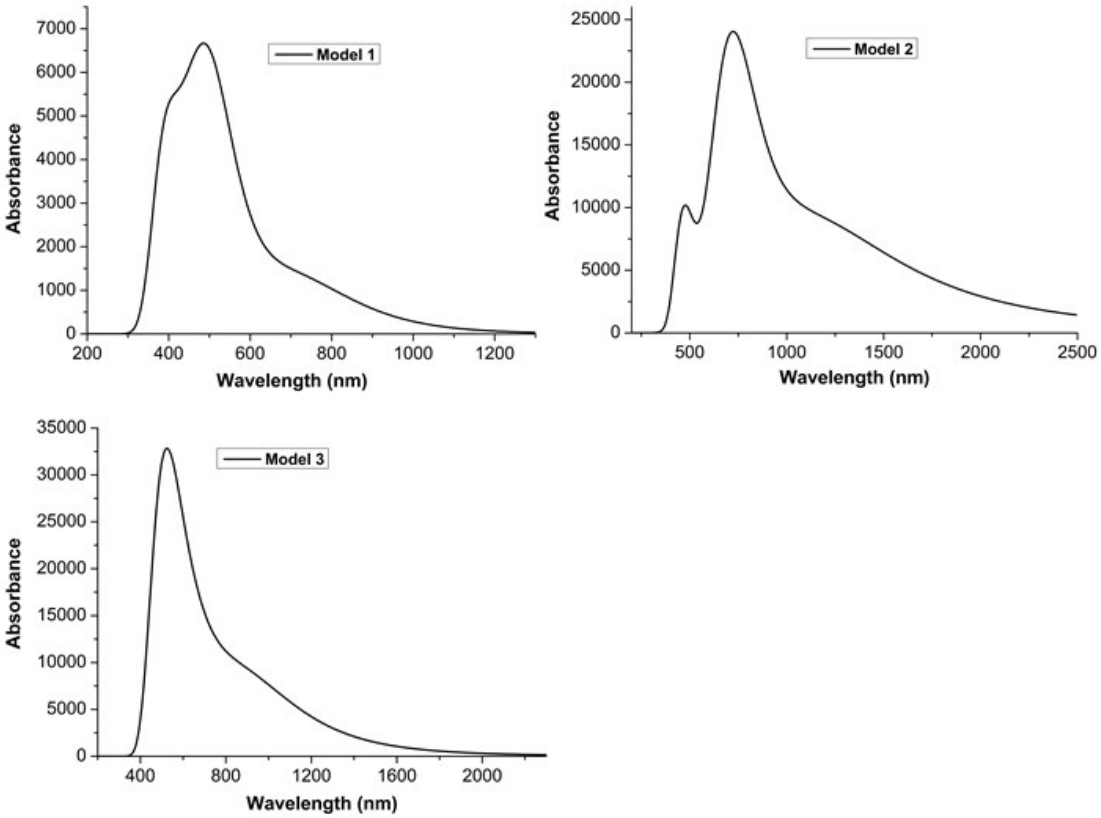

Figure S3. Predicted UV-Vis spectra of **Model 1**, **Model 2** and **Model 3**.

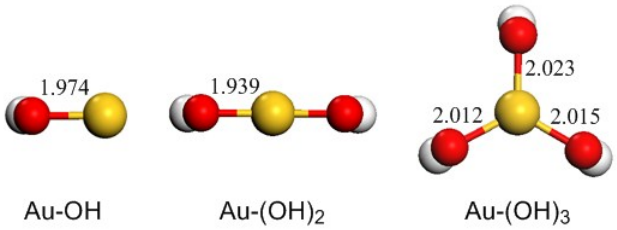

Figure S4. The Au-OH, Au-$(OH)_2$ and Au-$(OH)_3$ molecules are calculated in a cubic box of 20*20*20 Å. Copyright from ref. 54

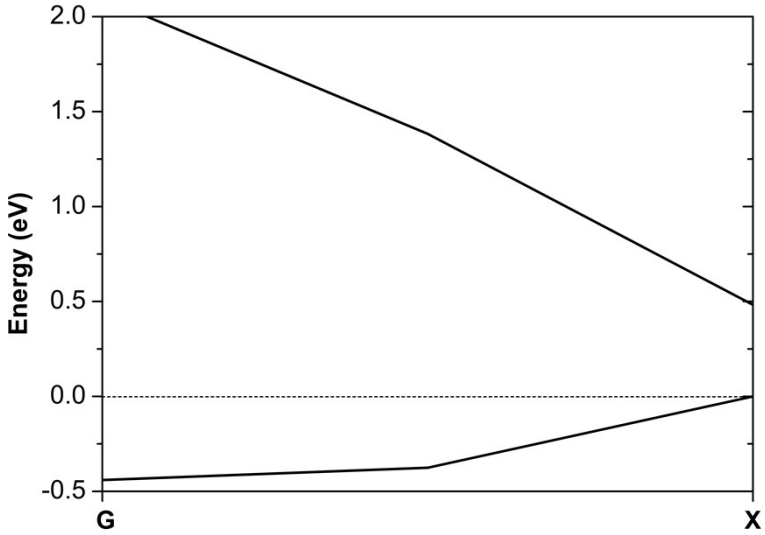

Figure S5. The calculated band structure of the 1D-IMGW by PBE0 hybrid density functional. The Fermi level is set at zero

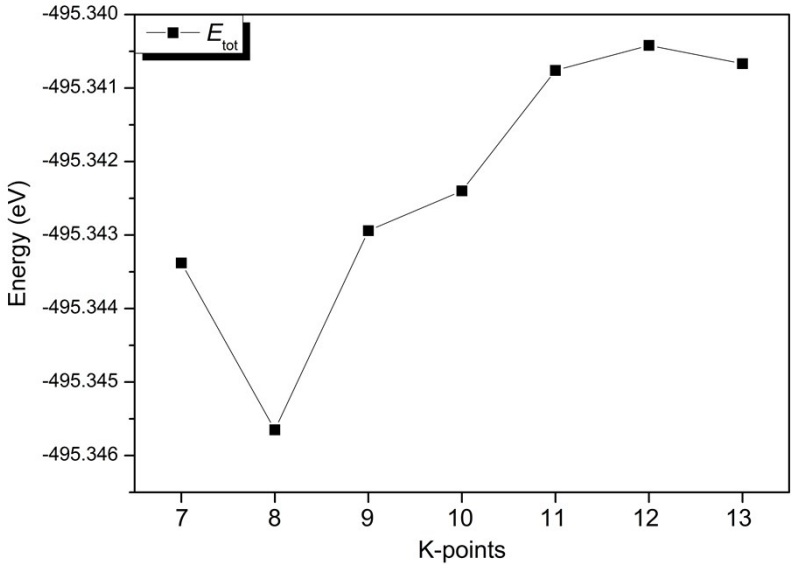

Figure S6. The calculated total energies of the 1D-IMGW using different k-points 7x1x1, 8x1x1, 9x1x1, 10x1x1, 11x1x1, 12x1x1, and 13x1x1 respectively.

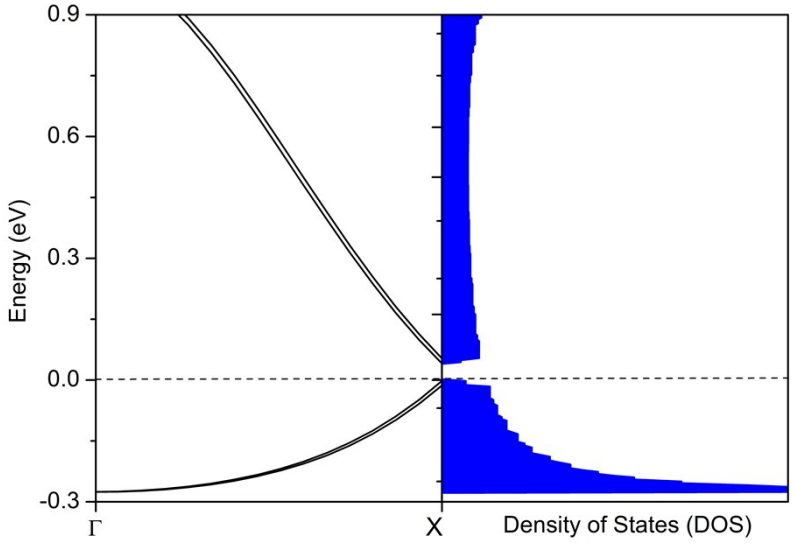

Figure S7. The enlarged band structure (left) and density of states (right) of the 1D-IMGW calculated by PBE. The Fermi level is set at zero.

Table S1. The calculated bond lengths of Au-Au (D_{Au-Au}) in **Model 1** using different density functional theory (DFT) of B3LYP, CAM-B3LYP, BP86 and PBE.

DFT	B3LYP	CAM-B3LYP	BP86	PBE
D_{Au-Au}	3.102	3.067	2.940	2.941

Table S2. Bader charges for Au atoms in the center of corrole rings (Au_c) and between the corrole rings (Au_i) and Au-OH, Au-$(OH)_2$ and Au-$(OH)_3$ molecules in the cubic box of 20*20*20 Å.

Species	Au-O Bond length (Å)	Au Valence electron	Au Bader charge (e)
Au_c	---	10.033	0.967
		10.051	0.949
Au_i	---	11.131	-0.131
		11.141	-0.141
Au-OH	1.974	10.681	0.319
Au-$(OH)_2$	1.939	10.412	0.588
Au-$(OH)_3$	2.012, 2.023, 2.015	10.079	0.921

ECP Valance electrons used in the calculations: Au ($d^{10}s^1$). Copyright from ref. 54