

Table S1. Effective U value (U_{ef}) versus the calculated MAE (in meV) of some systems with large MAE.

U_{ef}/eV	Re@Pc	Os-Os@Pc	Ir-Ir@Pc
0	20.72	40.67	47.21
0.5	21.10	60.99	92.38
1.0	10.64	107.96	50.03
1.5	17.67	73.88	46.63
2.0	N/A ^a	32.04	44.05

^a $U = 2$ eV leads to failure of SCF convergence for Re@Pc.