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$U_{ef}/eV$	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 <sup>a</sup>	32.04	44.05

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

<sup>a</sup> U = 2 eV leads to failure of SCF convergence for Re@Pc.