Supplementary Materials

First-principles study of Ir_n (n = 3-5) clusters adsorbed on graphene and hexagonal boron nitride: structural and magnetic properties

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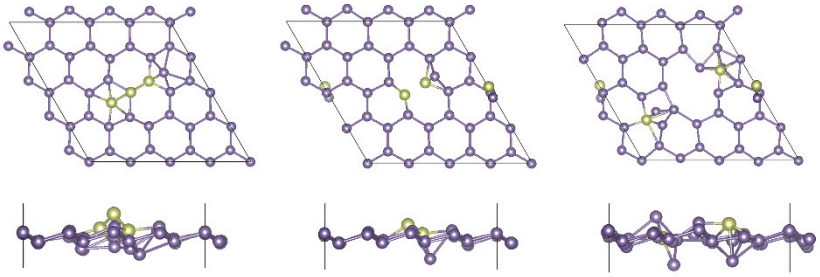

Figure S1 Three optimized configurations of Ir_3 on Germanene.

Table S1 The relative energies (in meV) of ferromagnetic (FM) and anti-ferromagnetic (AFM) states for the free–standing Ir_n and Ir_n on graphene and *h*BN substrates. We set the energy of FM (E_{FM}) state as zero.

n	Free standing		On graphene		On *h*BN	
	E_{FM}	E_{AFM}	E_{FM}	E_{AFM}	E_{FM}	E_{AFM}
3	0	0.0002	0	0.0114	0	0.0198
4	0	511.916	0	16.7884	0	255.587
5	0	0.0659	0	0.0182	0	0.0022