Electronic Supplementary Material (ESI) for Nanoscale

Supplementary Information

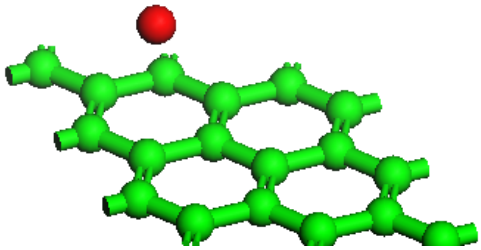

Table S1. Calculated binding energy of a metal atom (red sphere) located on the center of a hexagon of the graphene. Optimization of the structure is at the GGA/PBE level of theory.

	Li	Na	Mg	Al	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu
E_b(eV)	0.97	0.82	0.17	1.00	2.1	1.32	1.40	0.27	0.29	0.52	0.57	0.88	0.22

Figure S1. A plot of the first, second, and third narrowest AGNRs and ZGNRs.

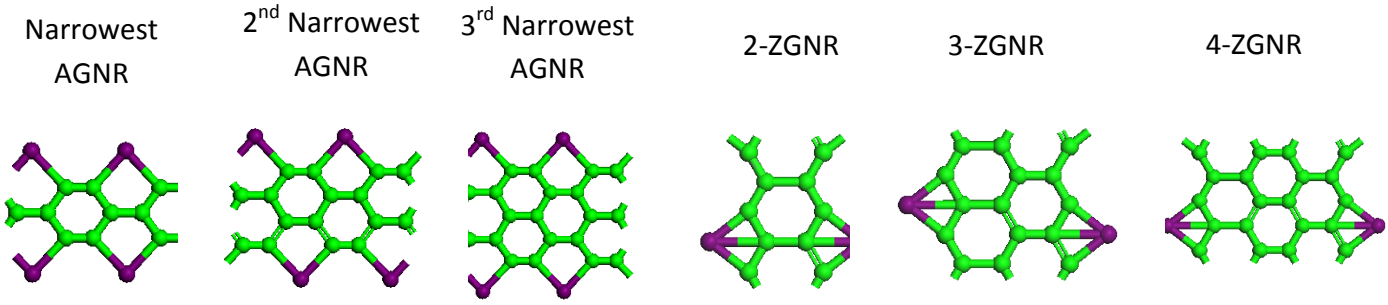

Figure S2. Snapshot of a Sc atom (per supercell), initially 4 Å away from an unpassivated edge of 2-ZGNR at 300 K (left panel). At the end of 0.2ps quantum molecular dynamics simulations the Sc atom binds to the edge of 2-ZGNR and the system become the 2-ZGNR>Sc/2 (right panel).