Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Tunnel Barrier to Spin Filter: Electronic Transport Characteristics of Transition Metal Atom Encapsulated in Smallest Cadmium Telluride Cage

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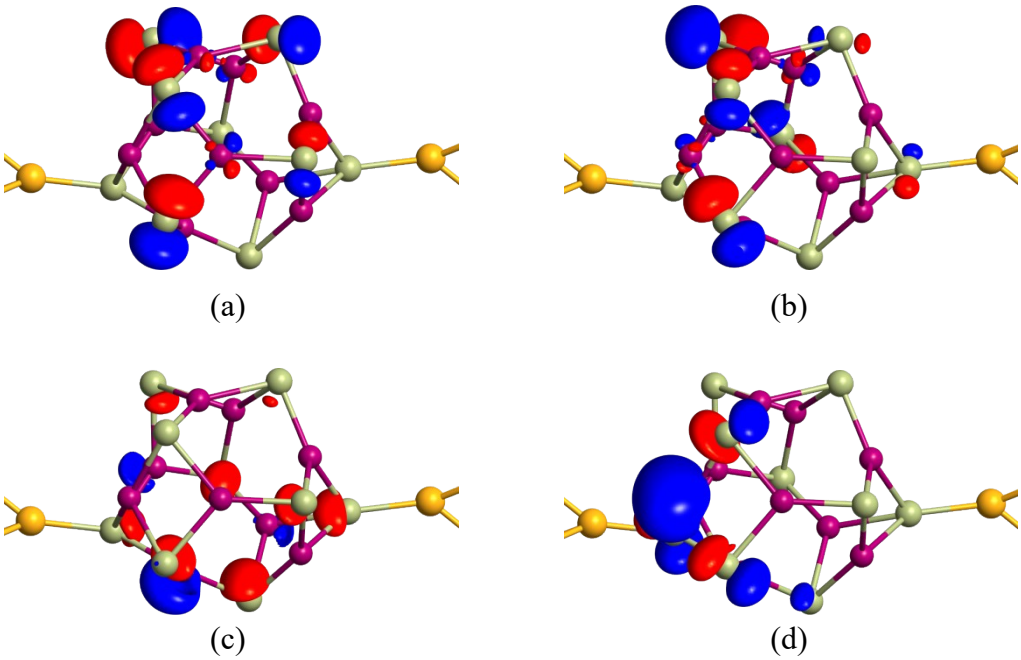


Figure S1. Eigenstates corresponding to (a) HOMO-1, (b) HOMO, (c) LUMO and (d) LUMO+1 energies of sandwiched Cd_9Te_9 cluster [iso value: 0.1]. The results are identical for up and down spins, as expected. The Cd atoms are in magenta, Te in olive green and Au in yellow.

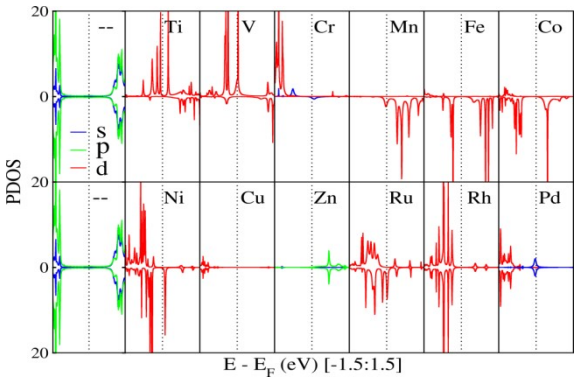
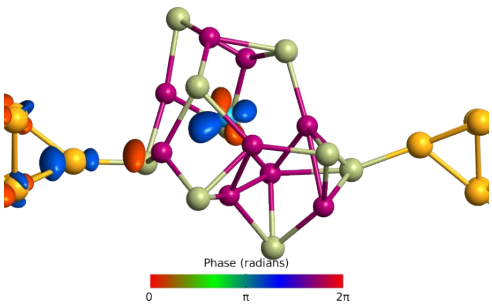
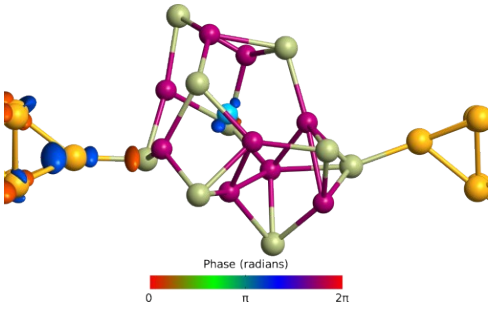


Figure S2. Spin resolved, orbital projected (TM *s*, *p*, *d*) device density of states for TM atom(s) encapsulated in Cd_9Te_9 cage sandwiched between Au (111) electrodes. Plots in the 1st column (Cd *s* and Te *p*) correspond to a bare cage, a reference device. For each plot, energy ranges from -1.5 eV to 1.5 eV about the respective Fermi energy.

Ti

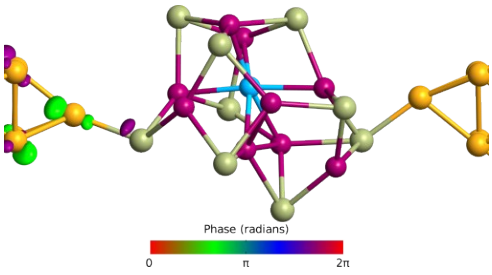


(a)

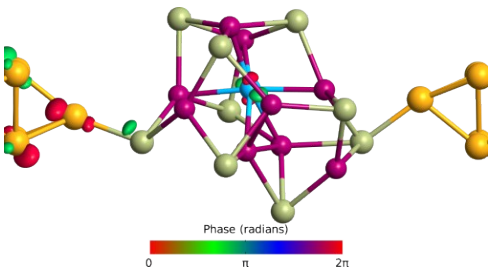


(b)

Fe

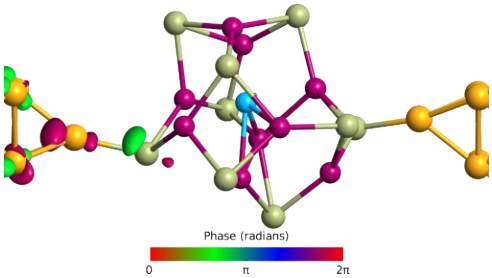


(c)

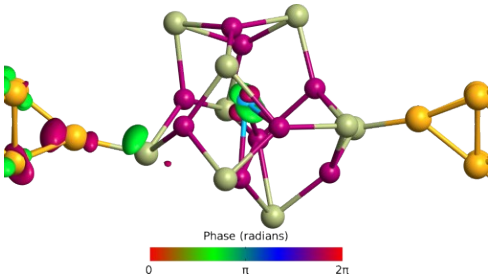


(d)

Co

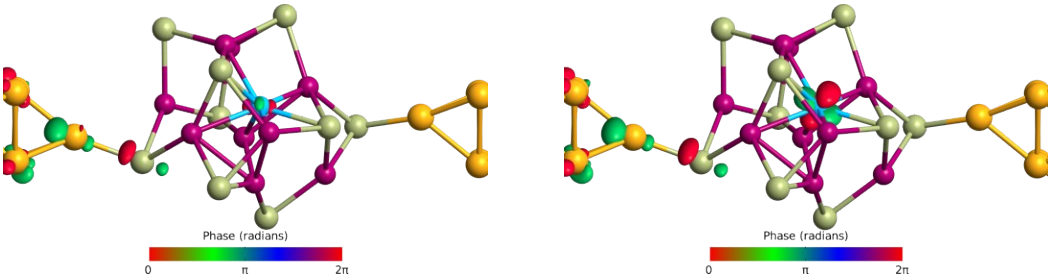


(e)



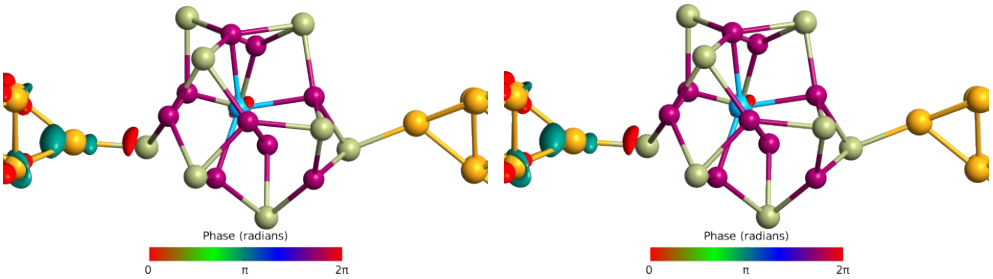
(f)

Ni



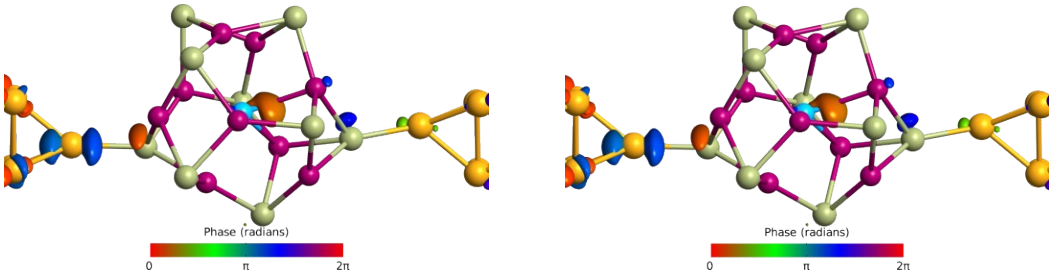
(g) (h)

Cu



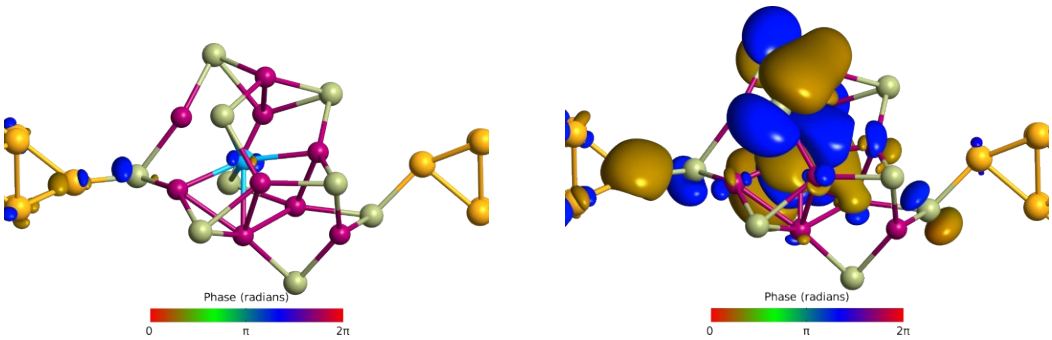
(i) (j)

Zn



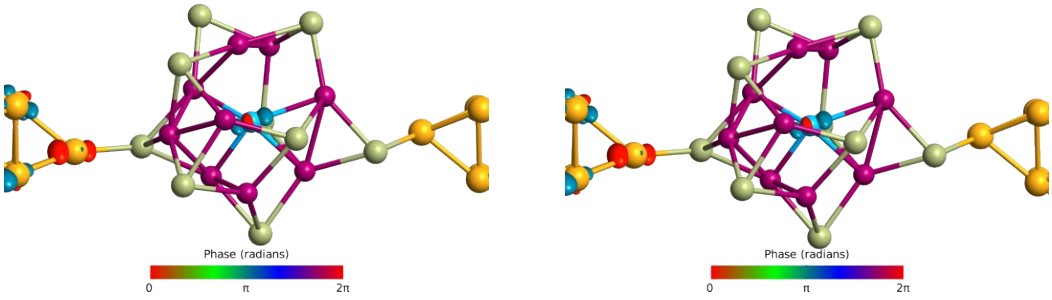
(k) (l)

Ru



(m) (n)

Rh



(o) (p)

Figure S3: Transmission eigenstates for the device with respective TM atom encapsulated in Cd_9Te_9 cage at Fermi level for (a) up and (b) down spins. (iso value: 0.4).

TM	Transmission Eigenvalues (in eV) × 10^{-2}	
	Up spin	Down spin
Ti	0.573	3.640
V	1.728	2.340
Cr	6.335	29.57
Mn	3.819	18.66
Fe	0.634	1.090
Co	1.368	2.326
Ni	0.205	0.256
Cu	1.560	1.560
Zn	43.24	43.24
Ru	0.742	18.00
Rh	0.192	0.193
Pd	6.165	6.180

Table ST1: Transmission eigenvalues for device of TM atom(s) encapsulated in Cd_9Te_9 cage at Fermi level for up and down spins.

TM	Isolated Cluster				In Device				Spin Polarization change (%) from cluster to device
	Total charge (↑ + ↓)			Difference (↑ - ↓)	Total charge (↑ + ↓)			Difference (↑ - ↓)	
	Cd	Te	TM	TM (A)	Cd	Te	TM	TM (B)	$100(A-B)/B$
CdTe(12,6)	11.77	6.22	-	-	11.78	6.17	-	-	--
Ti(4)	11.79	6.20	4.06	1.90	11.79	6.16	4.07	2.20	-15.8
V(5)	11.81	6.21	4.83	3.73	11.81	6.17	4.89	3.44	8.0
Cr(6)	11.84	6.20	5.64	5.17	11.85	6.15	5.64	5.02	2.9
Mn(7)	11.82	6.20	6.86	4.89	11.83	6.15	6.85	4.65	4.8
Fe(8)	11.80	6.20	7.93	3.63	11.81	6.16	7.88	3.28	9.8
Co(9)	11.82	6.19	8.92	2.48	11.81	6.16	8.97	2.17	12.5
Ni(10)	11.82	6.19	9.92	1.37	11.81	6.17	9.93	0.65	52.1
Cu(11)	11.78	6.18	11.34	0.00	11.78	6.16	11.36	0.00	0.0
Zn(12)	11.79	6.20	12.04	0.00	11.80	6.15	12.06	0.00	0.0
Ru(8)	11.78	6.19	8.27	1.97	11.77	6.14	8.52	0.65	66.7
Rh(9)	11.77	6.19	9.36	0.67	11.76	6.15	9.47	0.00	99.7
Pd(10)	11.74	6.20	10.52	0.00	11.74	6.16	10.67	0.00	0.0

Table ST2: Total electronic population on each atom in TM encapsulated Cd_9Te_9 cluster in isolated form and as a part of device. Total charge is addition of up and down spins, whereas the difference of the up and down spins shows the extent of spin polarization. The % change in spin polarization is the difference in the up and down spin populations of the TM atoms. The numbers are obtained from Mulliken analysis.