Supporting Information

Optical Properties and Quasiparticle Band Gaps of Transition-Metal Atoms Encapsulated by Silicon Cages

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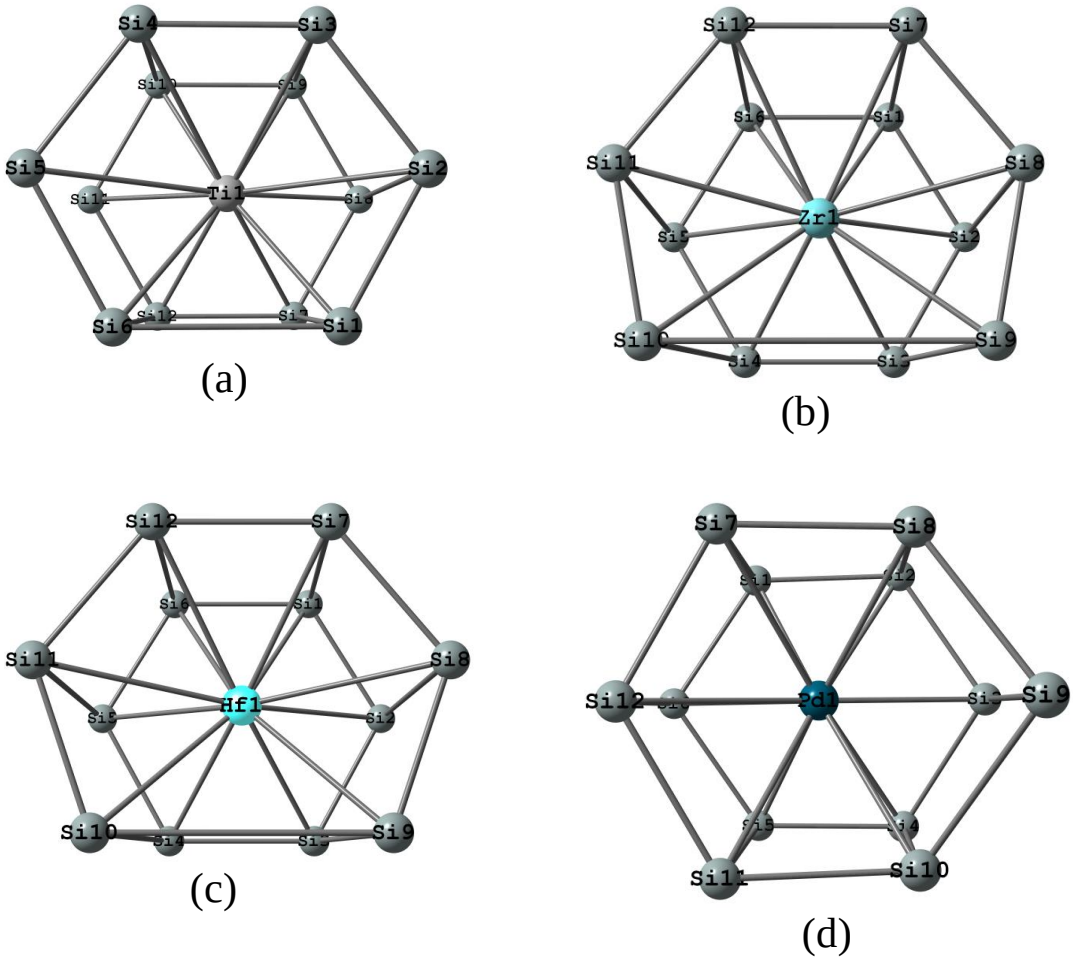

Figure S1. Illustration of some optimized geometries for the distorted M@Si_{12} clusters: Ti@Si_{12} (a), Zr@Si_{12} (b), Hf@Si_{12} (c), and Pd@Si_{12} (d).

Table S1. Atomic Coordinates of the $TiSi_{12}$ cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	5.17746	6.90445	6.48279
Si	5.52670	9.19602	6.31379
Si	7.80744	9.84675	6.27698
Si	9.67769	8.42687	6.27313
Si	9.65747	6.05509	6.30633
Si	7.54391	5.10382	6.47745
Si	5.24851	6.52027	8.81722
Si	5.55143	8.86621	8.75070
Si	7.72499	9.78052	8.65045
Si	9.64186	8.31905	8.64623
Si	9.33851	5.98024	8.74401
Si	7.15581	5.06870	8.81244
Ti	7.44814	7.43199	7.44851

Table S2. Atomic Coordinates of the $CrSi_{12}$ cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	5.34546	6.59257	6.35439
Si	5.63694	8.91215	6.35426
Si	7.79142	9.81966	6.35431
Si	9.65451	8.40742	6.35435
Si	9.36307	6.08784	6.35431
Si	7.20857	5.18036	6.35426
Si	5.34531	6.59254	8.72264
Si	5.63668	8.91240	8.72253
Si	7.79146	9.81996	8.72254
Si	9.65470	8.40747	8.72259
Si	9.36329	6.08761	8.72257
Si	7.20853	5.18001	8.72250
Cr	7.50000	7.50000	7.53879

Table S3. Atomic Coordinates of the ZrSi12 cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	5.47563	6.77735	6.57087
Si	5.68433	9.11925	6.20069
Si	7.91090	9.96318	6.35543
Si	9.76854	8.55478	6.35602
Si	9.56297	6.18224	6.19802
Si	7.36494	5.34806	6.57204
Si	5.27833	6.53384	8.91797
Si	5.20737	8.90133	8.65804
Si	6.95649	10.39292	8.48342
Si	10.44795	7.74908	8.48097
Si	9.47865	5.66430	8.65508
Si	7.18220	5.08586	8.91827
Zr	7.68155	7.72780	7.93322

Table S4. Atomic Coordinates of the $MoSi_{12}$ cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	5.30910	6.57730	6.33914
Si	5.60540	8.93601	6.33908
Si	7.79631	9.85870	6.33910
Si	9.69088	8.42269	6.33912
Si	9.39460	6.06397	6.33911
Si	7.20368	5.14131	6.33908
Si	5.30884	6.57725	8.73781
Si	5.60518	8.93627	8.73774
Si	7.79640	9.85903	8.73776
Si	9.69116	8.42276	8.73779
Si	9.39480	6.06374	8.73777
Si	7.20359	5.14096	8.73774
Mo	7.49999	7.50000	7.53880

Table S5. Atomic Coordinates of the RuSi12 cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	5.33398	6.58778	6.34838
Si	5.62703	8.91963	6.34824
Si	7.79299	9.83193	6.34828
Si	9.66597	8.41220	6.34834
Si	9.37299	6.08034	6.34828
Si	7.20701	5.16811	6.34825
Si	5.33384	6.58774	8.72852
Si	5.62672	8.91992	8.72840
Si	7.79299	9.83223	8.72843
Si	9.66618	8.41227	8.72848
Si	9.37323	6.08010	8.72844
Si	7.20699	5.16773	8.72839
Ru	7.49999	7.50000	7.53961

Table S6. Atomic Coordinates of the $PdSi_{12}$ cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	5.39778	6.62107	6.33486
Si	5.67586	8.94447	6.24426
Si	7.84649	9.91033	6.63529
Si	9.69825	8.42194	6.24373
Si	9.37432	6.10472	6.33630
Si	7.21386	5.03722	6.49188
Si	5.27690	6.65827	8.69302
Si	5.67795	8.99080	8.59225
Si	7.86589	10.04940	9.04541
Si	9.70834	8.46519	8.59175
Si	9.49883	6.10791	8.69486
Si	7.23611	5.22012	8.90092
Pd	7.52925	7.46855	7.49552

Table S7. Atomic Coordinates of the $HfSi_{12}$ cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	5.41059	6.70780	6.49562
Si	5.66167	9.06446	6.27899
Si	7.87373	9.96768	6.29607
Si	9.78109	8.52175	6.29579
Si	9.50978	6.14790	6.27706
Si	7.30865	5.26944	6.49509
Si	5.29500	6.55870	8.87406
Si	5.23991	8.95682	8.73173
Si	7.20002	10.18421	8.57469
Si	10.17352	7.92977	8.57368
Si	9.51981	5.71127	8.72956
Si	7.19610	5.11642	8.87351
Hf	7.63006	7.66379	7.80417

Table S8. Atomic Coordinates of the $OsSi_{12}$ cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	5.33128	6.58663	6.34542
Si	5.62466	8.92141	6.34527
Si	7.79333	9.83484	6.34532
Si	9.66867	8.41335	6.34538
Si	9.37536	6.07856	6.34531
Si	7.20666	5.16520	6.34529
Si	5.33130	6.58666	8.73162
Si	5.62449	8.92160	8.73148
Si	7.79332	9.83497	8.73151
Si	9.66873	8.41335	8.73157
Si	9.37547	6.07842	8.73152
Si	7.20666	5.16499	8.73148
Os	7.50000	7.50000	7.53886

Table S9. Atomic Coordinates of the $TiSi_{16}$ cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	10.70194	11.21594	7.50491
Si	7.76037	11.34614	9.34842
Si	8.83326	12.02109	11.52414
Si	11.25528	12.17391	11.43032
Si	12.28563	11.26659	9.34817
Si	10.70194	8.78406	7.50491
Si	8.83326	7.97892	11.52414
Si	9.95391	7.38724	9.34829
Si	11.25528	7.82609	11.43032
Si	7.48953	10.00000	11.43048
Si	8.59578	10.00000	7.50500
Si	12.33384	10.00000	11.52400
Si	9.95391	12.61276	9.34829
Si	10.00005	10.00000	12.56638
Si	7.76037	8.65386	9.34842
Si	12.28563	8.73341	9.34817
Ti	10.00001	10.00000	9.96687

Table S10. Atomic Coordinates of the $ZrSi_{16}$ cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	10.71290	11.23492	7.48196
Si	7.69212	11.38307	9.33286
Si	8.80682	12.06662	11.51474
Si	11.25541	12.17413	11.45977
Si	12.35128	11.30733	9.33250
Si	10.71290	8.76508	7.48196
Si	8.80682	7.93338	11.51474
Si	9.95650	7.31007	9.33267
Si	11.25541	7.82587	11.45977
Si	7.48906	10.00000	11.45966
Si	8.57360	10.00000	7.48244
Si	12.38697	10.00000	11.51421
Si	9.95650	12.68993	9.33267
Si	10.00038	10.00000	12.67027
Si	7.69212	8.61693	9.33286
Si	12.35128	8.69267	9.33250
Zr	9.99995	10.00000	9.96567

Table S11. Atomic Coordinates of the $HfSi_{16}$ cluster, optimized at the PW91-PAW level.

Atom	x	y	z
Si	10.71075	11.23123	7.48770
Si	7.70277	11.37751	9.33521
Si	8.81272	12.05633	11.51349
Si	11.25509	12.17360	11.45613
Si	12.34116	11.30098	9.33488
Si	10.71075	8.76878	7.48770
Si	8.81272	7.94367	11.51349
Si	9.95611	7.32201	9.33508
Si	11.25509	7.82641	11.45613
Si	7.48958	10.00000	11.45590
Si	8.57787	10.00000	7.48819
Si	12.37515	10.00000	11.51299
Si	9.95611	12.67799	9.33508
Si	10.00033	10.00000	12.65534
Si	7.70277	8.62248	9.33521
Si	12.34116	8.69902	9.33488
Hf	9.99987	10.00000	9.96384