

SUPPLEMENTARY MATERIALS

The Coordination of Lanthanide Atoms with Stone–Wales Defects on Graphene: A Cluster DFT Analysis Using ECP Pseudopotentials

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Table S1. The total energies E , HOMO, LUMO and HOMO-LUMO gap energies for the isolated components (Ln atoms and SWG model) and their SWG + Ln complexes, as well as single-point energies of the distorted SWG clusters after removing Ln atom (SWG + Ln – Ln).

	E (Ha)	HOMO (eV)	LUMO (eV)	HOMO-LUMO gap (eV)
La	–31.4738454	–3.290	–2.984	0.306
Ce	–474.9214614	–2.745	–2.542	0.203
Pr	–516.8949712	–2.595	–1.825	0.770
Nd	–561.3384977	–3.067	–1.761	1.306
Pm	–608.3343374	–3.223	–2.749	0.474
Sm	–658.0150384	–3.246	–3.436	–0.190
Eu	–710.4273537	–3.279	–1.628	1.651
Gd	–765.7852539	–1.769	–1.480	0.289
Dy	–895.6892451	–4.853	–2.844	2.009
Ho	–948.5235539	–2.758	–0.902	1.856
Er	–1015.5947880	–2.570	–0.710	1.860
Tm	–1085.9692219	–2.520	–1.883	0.637
Yb	–1159.6558901	–3.243	–0.376	2.867
Lu	–39.8872389	–4.153	–1.828	2.325
SWG	–2525.1698644	–4.663	–3.770	0.893
SWG + La	–2556.8290238	–3.358	–3.133	0.225
SWG + Ce	–3000.2516802	–3.380	–3.153	0.227
SWG + Pr	–3042.1984917	–3.398	–3.114	0.284
SWG + Nd	–3086.6356604	–3.600	–3.119	0.481
SWG + Pm	–3133.6274801	–3.387	–3.116	0.271
SWG + Sm	–3183.2266146	–3.638	–3.280	0.358
SWG + Eu	–3235.6339427	–4.114	–3.119	0.995
SWG + Gd	–3291.0350489	–4.111	–3.178	0.933
SWG + Dy	–3420.9872344	–4.634	–4.222	0.412
SWG + Ho	–3473.7721297	–3.741	–3.266	0.475
SWG + Er	–3540.7522861	–3.643	–3.261	0.382

SWG + Tm	−3611.1612737	−3.619	−3.310	0.309
SWG + Yb	−3684.8463059	−4.078	−3.348	0.730
SWG + Lu	−2565.1808529	−4.253	−3.539	0.714
SWG + La – La	−2525.1309227			
SWG + Ce – Ce	−2525.1296734			
SWG + Pr – Pr	−2525.1350625			
SWG + Nd – Nd	−2525.1353746			
SWG + Pm – Pm	−2525.1357688			
SWG + Sm – Sm	−2525.1392065			
SWG + Eu – Eu	−2525.1383448			
SWG + Gd – Gd	−2525.1491801			
SWG + Dy – Dy	−2525.1467161			
SWG + Ho – Ho	−2525.1374167			
SWG + Er – Er	−2525.1346624			
SWG + Tm – Tm	−2525.1363364			
SWG + Yb – Yb	−2525.1338783			
SWG + Lu – Lu	−2525.1368810			

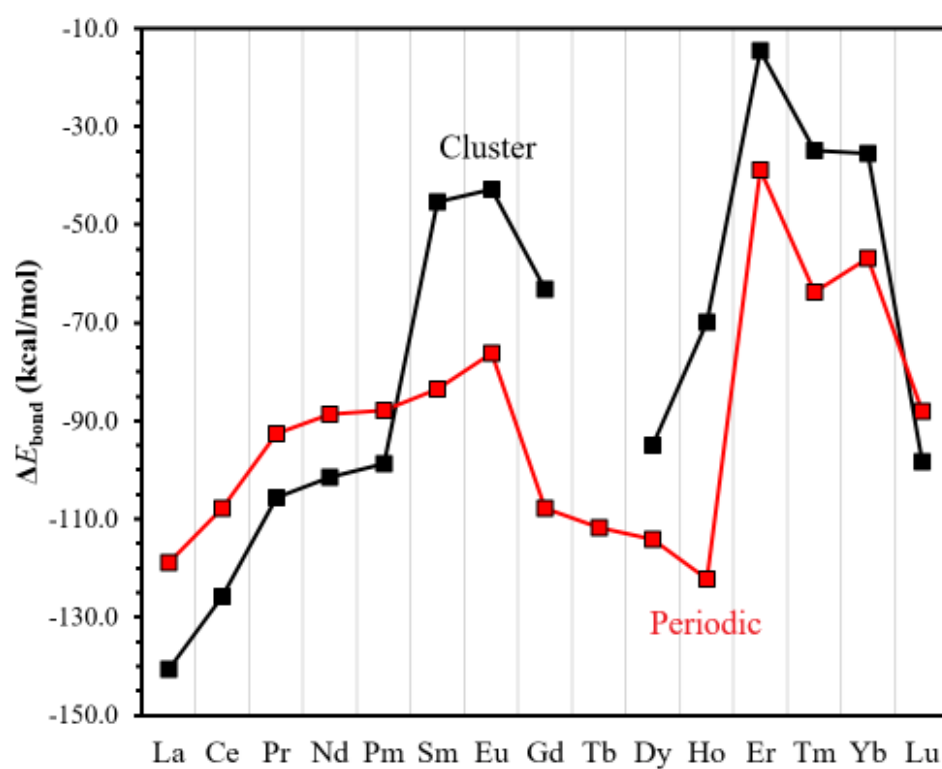


Figure S1. Comparison between the ΔE_{bond} values calculated for the cluster (present work) and periodic SWG models [39].

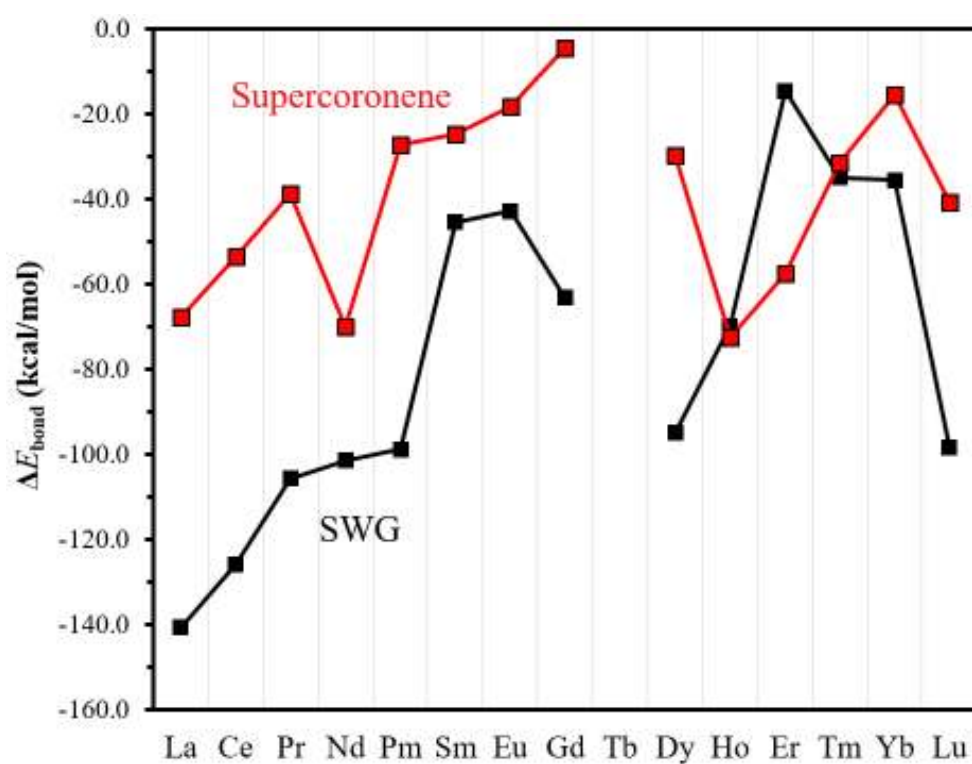


Figure S2. Comparison between the ΔE_{bond} values calculated for the SWG (present work) and supercoronene cluster models [41].