

Supplementary Information for ‘Structural and Optical properties of Be, Mg and Ca nanorods and nanodisks’

A. G. Chronis¹, F. I. Michos¹, C.S. Garoufalidis¹ and M. M. Sigalas¹

¹Department of Materials Science, University of Patras, GR-26504 Patras, Greece

In the following table, the binding energy (BE) per atom and the HOMO-LUMO (HL) gap, for the case of spherical Mg nanoparticles are presented. In table 2, the BE per atom and the HL gap, for the case of Mg nanorods are presented. The BE per atom and the HL gap, for the case of Mg nanodisks are presented at table 3. Finally, figure 1 shows a comparison between the three smaller spherical structures.

Table 1: The binding energy (BE) per atom and the HOMO-LUMO gap for the spherical Mg nanoparticles.

N atoms	BE per atom (eV)	HL gap (eV)
4	0.384	2.008
5	0.392	1.311
6	0.412	1.115
7	0.478	1.266
8	0.510	0.967
9	0.594	0.720
10	0.657	1.254
11	0.650	1.338
12	0.627	0.517
13	0.657	0.451
14	0.679	0.419
15	0.723	0.531
16	0.712	0.122
17	0.786	0.402
19	0.829	0.319
20	0.852	0.763
21	0.832	0.335
22	0.825	0.242
23	0.834	0.358
24	0.851	0.183
25	0.873	0.185
26	0.873	0.229

27	0.881	0.293
28	0.892	0.355
29	0.887	0.286
30	0.894	0.366
31	0.901	0.114
48	1.006	0.101
56	1.023	0.072
66	1.057	0.165
76	1.075	0.099

Table 2: The BE per atom and HL gap for the Mg nanorods.

N atoms	BE per atom (eV)	HL gap (eV)
24	0.806	0.043
36	0.936	0.058
48	0.985	0.031
72	1.044	0.096
96	1.082	0.101

Table 3: The BE per atom and HL gap for the Mg nanodisks.

N atoms	BE per atom (eV)	HL gap (eV)
24	0.806	0.043
54	0.941	0.048
96	1.016	0.052

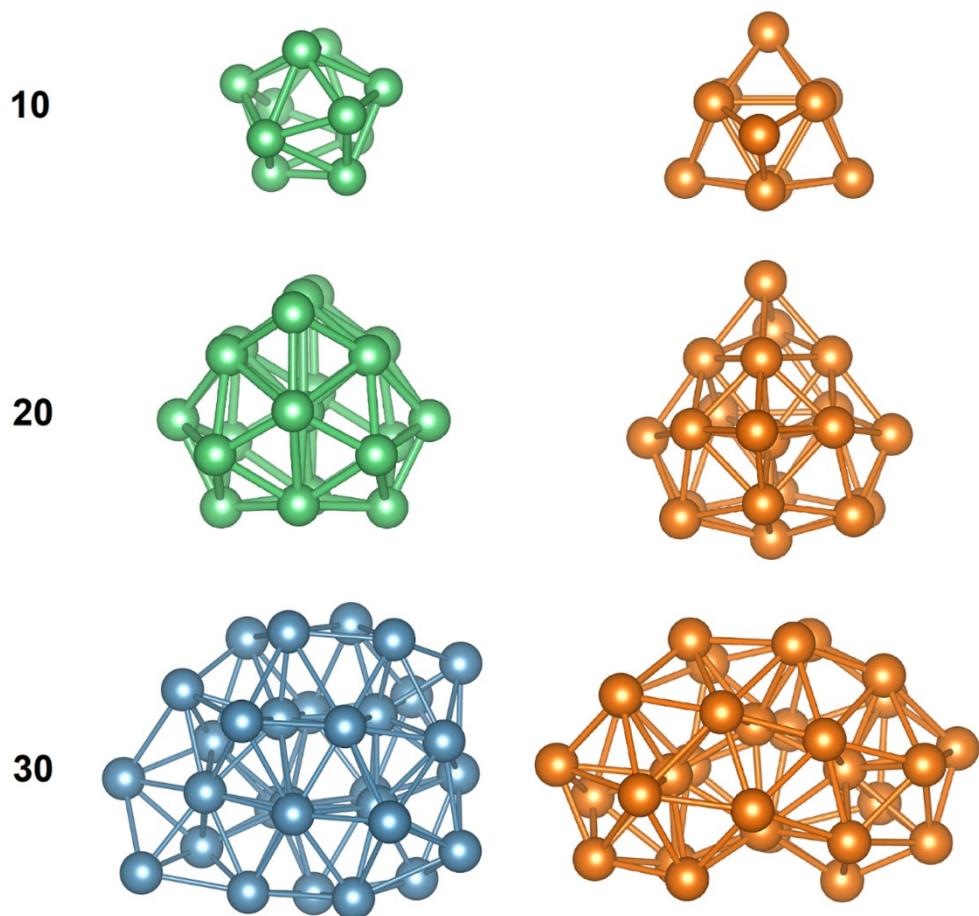


Figure 1: Some of the Be_n (green), Mg_n (orange) and Ca_n (blue) spherical structures, where $n=10, 20, 30$.