

Supplementary Information

Optical Properties of Aluminum Intercalated Magnesium Nanoparticle Square Array: A Computational Study

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Optimized atomic coordinates of single Mg NP

Mg	11.6000000	10.9237600	10.0000000
Mg	14.8000000	10.9237600	10.0000000
Mg	18.0000000	10.9237600	10.0000000
Mg	10.0000000	13.6950500	10.0000000
Mg	13.2000000	13.6950500	10.0000000
Mg	16.4000000	13.6950500	10.0000000
Mg	19.6000000	13.6950500	10.0000000
Mg	11.6000000	16.4663300	10.0000000
Mg	14.8000000	16.4663300	10.0000000
Mg	18.0000000	16.4663300	10.0000000
Mg	10.0000000	19.2376100	10.0000000
Mg	13.2000000	19.2376100	10.0000000
Mg	16.4000000	19.2376100	10.0000000
Mg	19.6000000	19.2376100	10.0000000
Mg	10.0000000	10.0000000	12.6050000
Mg	11.6000000	10.9237600	15.2100000
Mg	13.2000000	10.0000000	12.6050000
Mg	14.8000000	10.9237600	15.2100000
Mg	16.4000000	10.0000000	12.6050000
Mg	18.0000000	10.9237600	15.2100000
Mg	19.6000000	10.0000000	12.6050000
Mg	10.0000000	13.6950500	15.2100000
Mg	11.6000000	12.7712800	12.6050000
Mg	13.2000000	13.6950500	15.2100000
Mg	14.8000000	12.7712800	12.6050000
Mg	16.4000000	13.6950500	15.2100000
Mg	18.0000000	12.7712800	12.6050000
Mg	19.6000000	13.6950500	15.2100000
Mg	10.0000000	15.5425700	12.6050000
Mg	11.6000000	16.4663300	15.2100000
Mg	13.2000000	15.5425700	12.6050000
Mg	14.8000000	16.4663300	15.2100000
Mg	16.4000000	15.5425700	12.6050000
Mg	18.0000000	16.4663300	15.2100000
Mg	19.6000000	15.5425700	12.6050000
Mg	10.0000000	19.2376100	15.2100000
Mg	11.6000000	18.3138500	12.6050000

Mg	13.2000000	19.2376100	15.2100000
Mg	14.8000000	18.3138500	12.6050000
Mg	16.4000000	19.2376100	15.2100000
Mg	18.0000000	18.3138500	12.6050000
Mg	19.6000000	19.2376100	15.2100000
Mg	10.0000000	10.0000000	17.8150000
Mg	11.6000000	10.9237600	20.4200000
Mg	13.2000000	10.0000000	17.8150000
Mg	14.8000000	10.9237600	20.4200000
Mg	16.4000000	10.0000000	17.8150000
Mg	18.0000000	10.9237600	20.4200000
Mg	19.6000000	10.0000000	17.8150000
Mg	10.0000000	13.6950500	20.4200000
Mg	11.6000000	12.7712800	17.8150000
Mg	13.2000000	13.6950500	20.4200000
Mg	14.8000000	12.7712800	17.8150000
Mg	16.4000000	13.6950500	20.4200000
Mg	18.0000000	12.7712800	17.8150000
Mg	19.6000000	13.6950500	20.4200000
Mg	10.0000000	15.5425700	17.8150000
Mg	11.6000000	16.4663300	20.4200000
Mg	13.2000000	15.5425700	17.8150000
Mg	14.8000000	16.4663300	20.4200000
Mg	16.4000000	15.5425700	17.8150000
Mg	18.0000000	16.4663300	20.4200000
Mg	19.6000000	15.5425700	17.8150000
Mg	10.0000000	19.2376100	20.4200000
Mg	11.6000000	18.3138500	17.8150000
Mg	13.2000000	19.2376100	20.4200000
Mg	14.8000000	18.3138500	17.8150000
Mg	16.4000000	19.2376100	20.4200000
Mg	18.0000000	18.3138500	17.8150000
Mg	19.6000000	19.2376100	20.4200000

Figure S1

