Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for

The Effect of Particle Size on the Optical and Electronic Properties of Magnesium Oxide Nanoparticles

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Table S1 Occupied (–IP) and unoccupied (–EA) edge states, fundamental gap (Δ_F), optical gap (Δ_O) and exciton binding energy (EBE) values of $(MgO)_{32}$ as calculated using BSE/G_0W_0(AC)/def2-TZVPP and BSE/evGW(AC)/def2-TZVPP starting from PBE rather than B3LYP orbitals. The geometry used was that obtained using B3LYP/def2-TZVPP.

MgO	G_0W_0@PBE					evGW@PBE				
	–IP	–EA	Δ_F	Δ_O	EBE	–IP	–EA	Δ_F	Δ_O	EBE
32 (4:4:4)	-7.018	-0.610	6.41	3.312	3.10	-8.226	-0.245	7.98	4.815	3.17

Table S2 Occupied (–IP) and unoccupied (–EA) edge states, fundamental gap (Δ_F), optical gap (Δ_O) and exciton binding energy (EBE) values of $(MgO)_{18}$ as calculated by the different method combinations and the def2-TZVPP basis-set.

MgO	G_0W_0					evGW				
	–IP	–EA	Δ_F	Δ_O	EBE	–IP	–EA	Δ_F	Δ_O	EBE
18 (3:3:3)	-6.807	-0.892	5.92	3.434	2.48	-7.481	-0.670	6.81	4.299	2.51

Table S3 Occupied (–IP) and unoccupied (–EA) edge states, fundamental gap (Δ_F), optical gap (Δ_O) and exciton binding energy (EBE) values of the alternative structure for $(MgO)_{27}$ as calculated by the different method combinations and the def2-SVP basis-set.

MgO	G_0W_0					evGW				
	–IP	–EA	Δ_F	Δ_O	EBE	–IP	–EA	Δ_F	Δ_O	EBE
27 (5:3:3)	-6.925	-0.385	6.54	3.653	2.89	-7.563	-0.159	7.40	4.482	2.92

Table S4 Occupied (–IP) and unoccupied (–EA) edge states, fundamental gap (Δ_F), optical gap (Δ_O) and exciton binding energy (EBE) values of $(CaO)_{32}$ and $(SrO)_{32}$ cubes predicted using BSE/G_0W_0(AC)/def2-TZVPP and BSE/evGW(AC)/def2-TZVPP starting from PBE rather than B3LYP orbitals. The geometry used was that obtained using B3LYP/def2-TZVPP.

	G_0W_0					evGW				
	–IP	–EA	Δ_F	Δ_O	EBE	–IP	–EA	Δ_F	Δ_O	EBE
CaO (4:4:4)	-5.545	-0.151	5.39	2.432	2.96	-6.562	0.114	6.68	3.929	2.75
SrO (4:4:4)	-5.051	-0.200	4.85	2.293*	2.56	-6.069	0.061	6.13	3.510*	2.62

* The lowest excited-state for $(SrO)_{32}$ as calculated using BSE/G_0W_0(AC)/def2-TZVPP and BSE/evGW(AC)/def2-TZVPP is symmetry forbidden. The 2.293 and 3.510 eV excitations, respectively, are the lowest optically allowed excitations, second lowest overall. The lowest BSE/G_0W_0(AC)/def2-TZVPP and BSE/evGW(AC)/def2-TZVPP excitation belongs to the A irrep for T_d and has an excitation energy of 2.277 eV and an EBE value of 2.57 eV and an excitation energy of 3.493 eV and an EBE value of 2.64 eV, respectively.

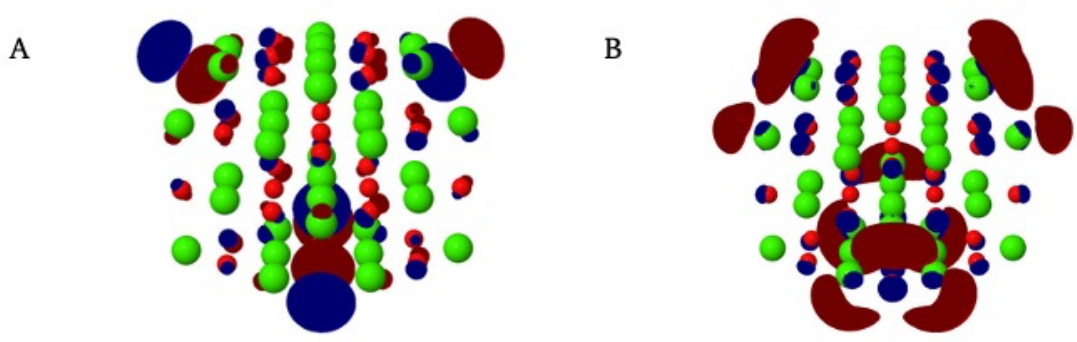

Fig. S1 Leading occupied (A) and unoccupied (B) natural transition orbitals for the lowest excitation of $(CaO)_{32}$. As the calculation was performed using the D_2 instead of the T_d point group, the triply degenerate T_2 excited state is described as a triplet of excited states of B1, B2 and B3 symmetry, the natural transition orbitals of only one is shown here.