

Supporting Information

for

Development of a charge-perturbed particle-in-a-sphere model for nanoparticle electronic structure

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Coordinates of the perturbations for the test cases

- Case 1a: P1(0,0,4.5); P2 (0,0,-4.5)
- Case 1b: P1(-1.2287,-2.3450,-3.6388); P2 (1.2287,2.3450,3.6388)
- Case 2: P1(0,4.5,0); P2 (0,-4.5,0); P3(4.5,0,0); P4 (-4.5,0,0)
- Case 3: P1(0,4.5,0); P2 (0,-4.5,0); P3(4.5,0,0); P4 (-4.5,0,0); P5(0,0,4.5); P6 (0,0,-4.5)
- Case 4: P1(0,4.5,0); P2 (0,-4.5,0); P3(4.5,0,0); P4 (-4.5,0,0); P5(3.18198,3.18198,0); P6 (3.18198, -3.18198,0); P7(-3.18198,-3.18198,0); P8 (-3.18198, 3.18198,0)
- Case 5: P1(0,4.5,0); P2 (0,-4.5,0); P3(4.5,0,0); P4 (-4.5,0,0); P5(0,0,4.5); P6 (0,0,-4.5); P7(-3.18198,-3.18198,0); P8 (-3.18198, 3.18198,0); P9(3.18198,3.18198,0); P10 (3.18198, -3.18198,0); P11(0,3.18198,3.18198); P12 (0,3.18198, -3.18198); P13(0,-3.18198,-3.18198); P14(0,-3.18198, 3.18198); P15(3.18198,0,3.18198); P16 (3.18198,0, -3.18198); P17(-3.18198,0,-3.18198); P18(-3.18198,0,3.18198)

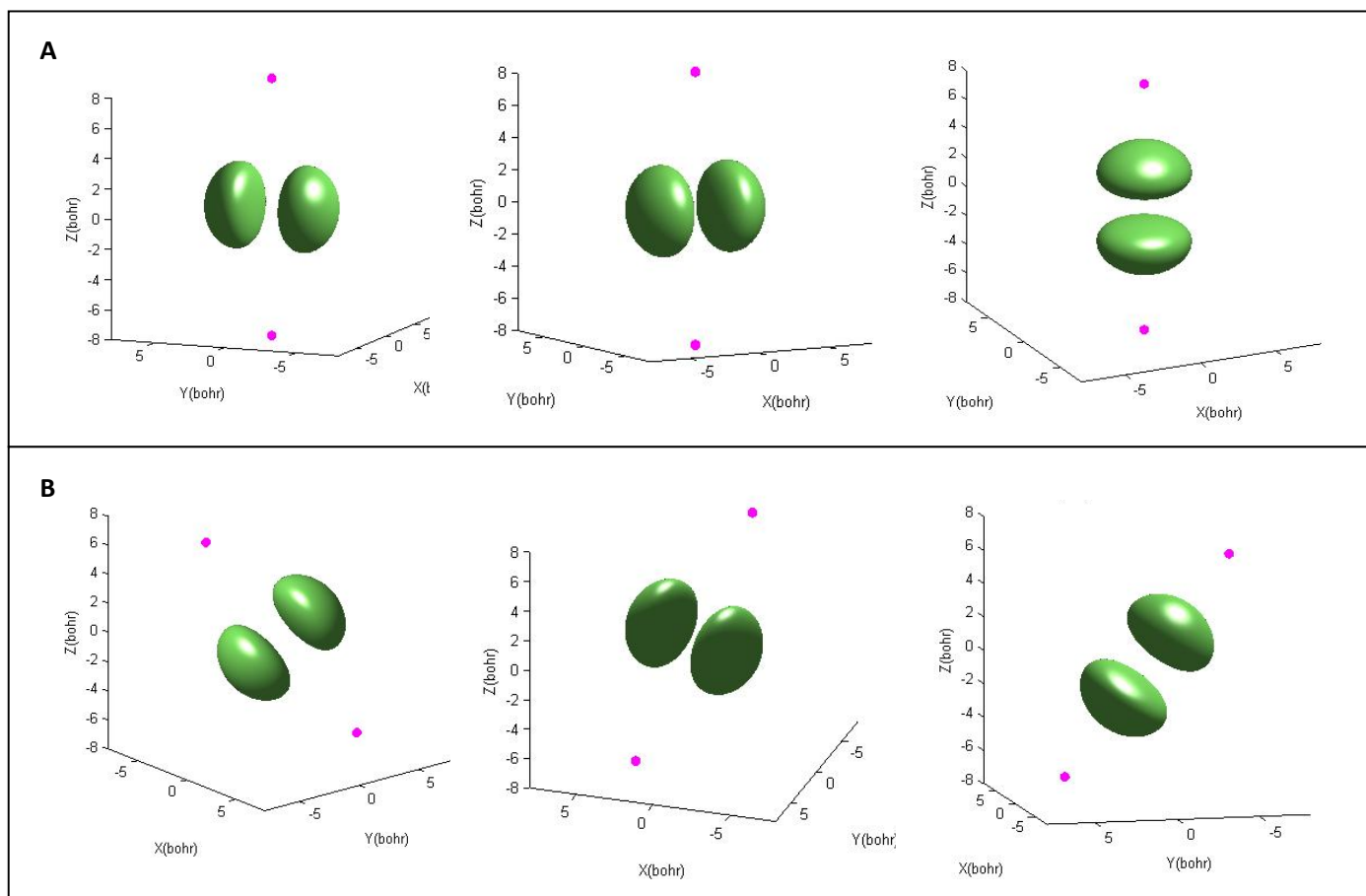


Figure S1: A) P orbitals of test case 1a and B) P orbitals of test case 1b. Green: Orbitals. Magenta: Point charge perturbations.