$C_{20}H_{10}$ Superatom States: a unique route for electron transport ?

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Computational Methodology: The structural and energetic analyses of the molecular systems described in this study were carried out with the B97-D dispersion enabled density functional,[S1,S2] using an ultrafine grid, together with the Def2-TZVPP basis set.[S3] Full geometry optimizations were performed and uniquely characterized via second derivatives (Hessian) analysis.

The calculations of the electronic properties of the gas phase molecules have been carried out at a DFT-LDA and DFT-PBE0 level with supercell geometries, plane wave basis sets and pseudopotentials using the quantum-espresso code[S4] The evaluation of quasi particle spectra have been performed within G_0W_0 framework, using the SAX code,[S5] with a Godby-Needs plasmon pole approximation[S6] for the energy dependence of the screened Coulomb potential. A cut-off of 45 ry was used for the electronic wave-function and the Fock operator and a cut-off of 2 ry for the evaluation of the polarizability. G_0W_0 quasiparticle energies have been obtained in a perturbation scheme exploiting both DFT-LDA[S7] and DFT-PBE0[S8] Kohn and Sham eigenvalues. A unit-cell of (25x25x25) Å, and the Martyna-Tuckerman method[S9] has been applied, both in DFT calculations and in the GW calculation, to avoid replica interactions.

S1. Grimme, S., *J. Comput. Chem.* **2006,** *27*, 1787-1799.
S2. Grimme, S., *J. Chem. Phys.* **2006,** *124*, 034108-034115.
S3. Weigend, F.; Ahlrichs, R. *Phys.Chem.Chem.Phys*., **2005**, *7,* 3297-3305.
S4. Giannozzi, P.; Baroni, S.; Bonini, N.; Calandra, M.; Car, R.; Cavazzoni, C.; Ceresoli, D.; Chiarotti, G. L.; Cococcioni, M.; Dabo, I.; Corso, A. D.; Gironcoli, S. d.; Fabris, S.; Fratesi, G.; Gebauer, R.; Gerstmann, U.; Gougoussis, C.; Kokalj, A.; Lazzeri, M.; Martin-Samos, L.; Marzari, N.; Mauri, F.; Mazzarello, R.; Paolini, S.; Pasquarello, A.; Paulatto, L.; Sbraccia, C.; Scandolo, S.; Sclauzero, G.; Seitsonen, A. P.; Smogunov, A.; Umari, P.; Wentzcovitch, R. M., *J. Phys.:Condens. Matter* **2009,** *21*, 395502.
S5. Martin-Samos, L.; Bussi, G., *Comp. Phys. Comm.* **2009,** *180*, 1416-1425.
S6. Godby, R.W.; Needs, R.J. *Phys. Rev. Lett.* **1989**, *62*, 1169.
S7. Perdew, J. P.; Zunger, A., *Phys. Rev. B* **1981,** *23*, 5048-5079.
S8. Ernzerhof, M.; Scuseria, G. E., *J. Chem. Phys.* **1999,** *110*, 5029-5035.
S9. Martyna, G.J.; Tuckerman, M.E. *J. Chem. Phys*., **1999**, *110* (6), 2810.