

Selective interface transparency in graphene nanoribbon based molecular junctions

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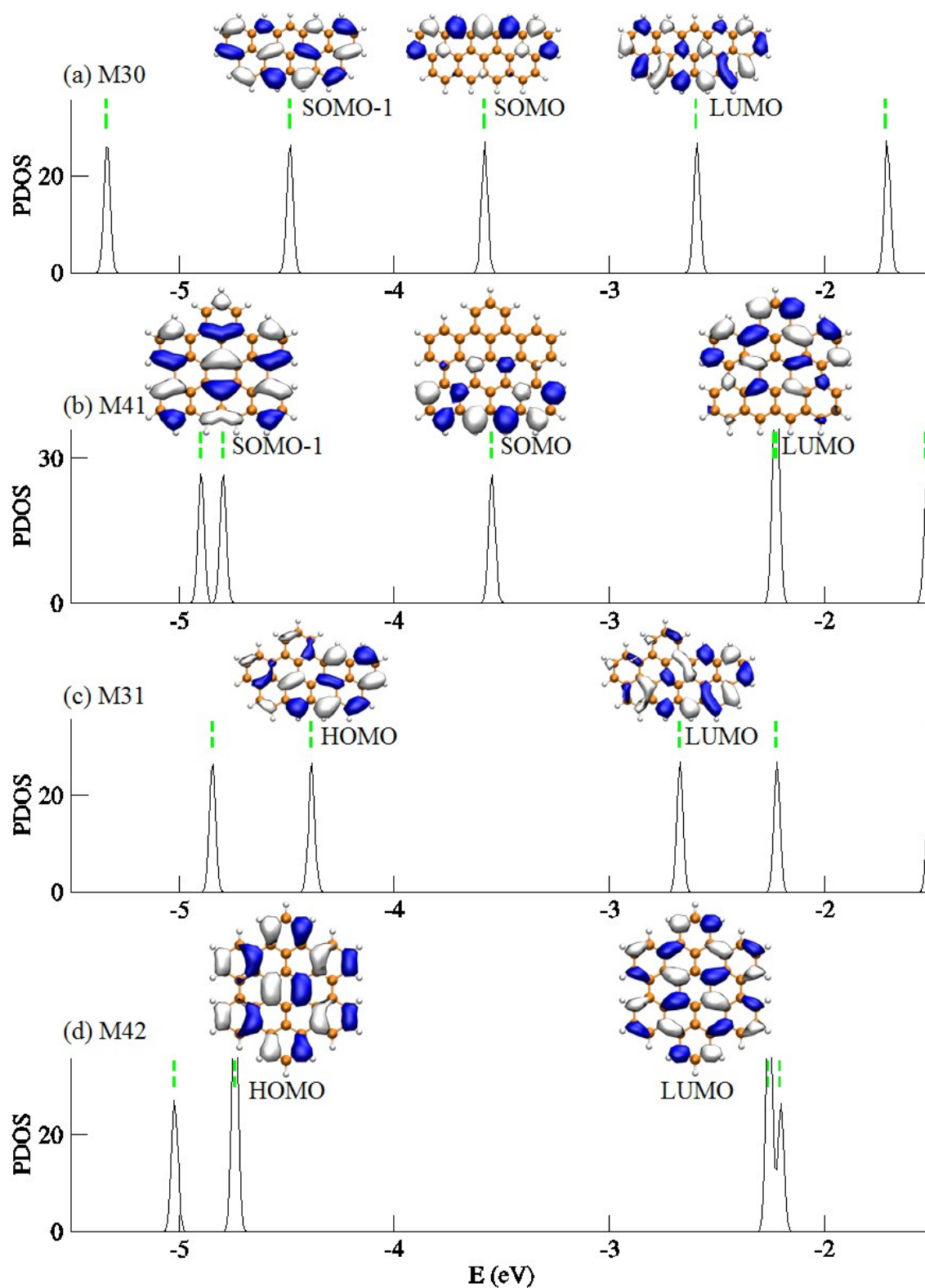


Fig. S1 Projected density of states for isolated M30, M41, M31 and M42. Selected orbital functions are shown at the top of each panel.

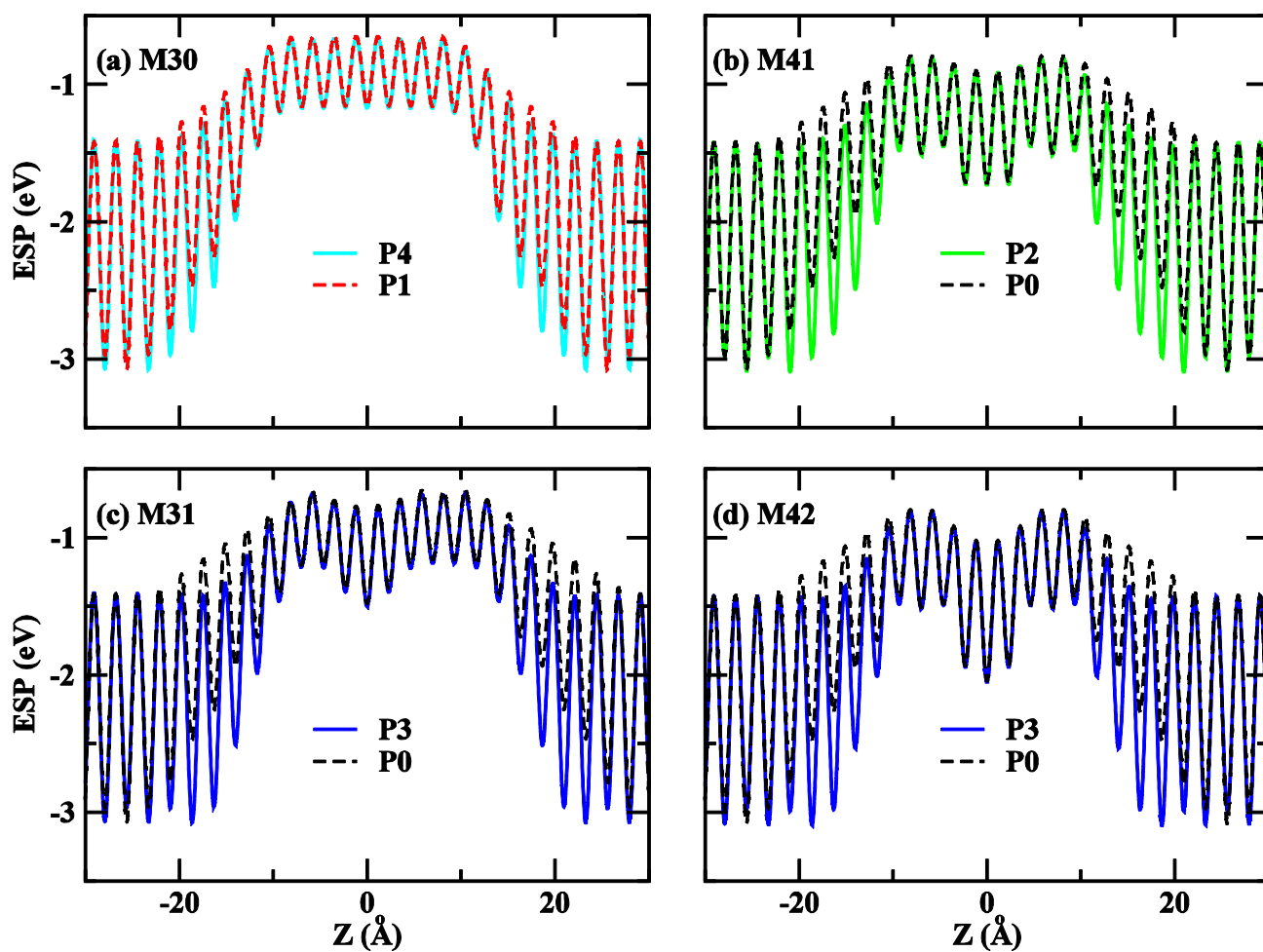


Fig. S2 Plane-averaged electrostatic potential for (a) S_{M30P4} , S_{M30P1} ; (b) S_{M41P2} , S_{M41P0} ; (c) S_{M31P3} , S_{M31P0} ; (d) S_{M42P3} , S_{M42P0} . The colors for each model correlate with those in Fig. 1.

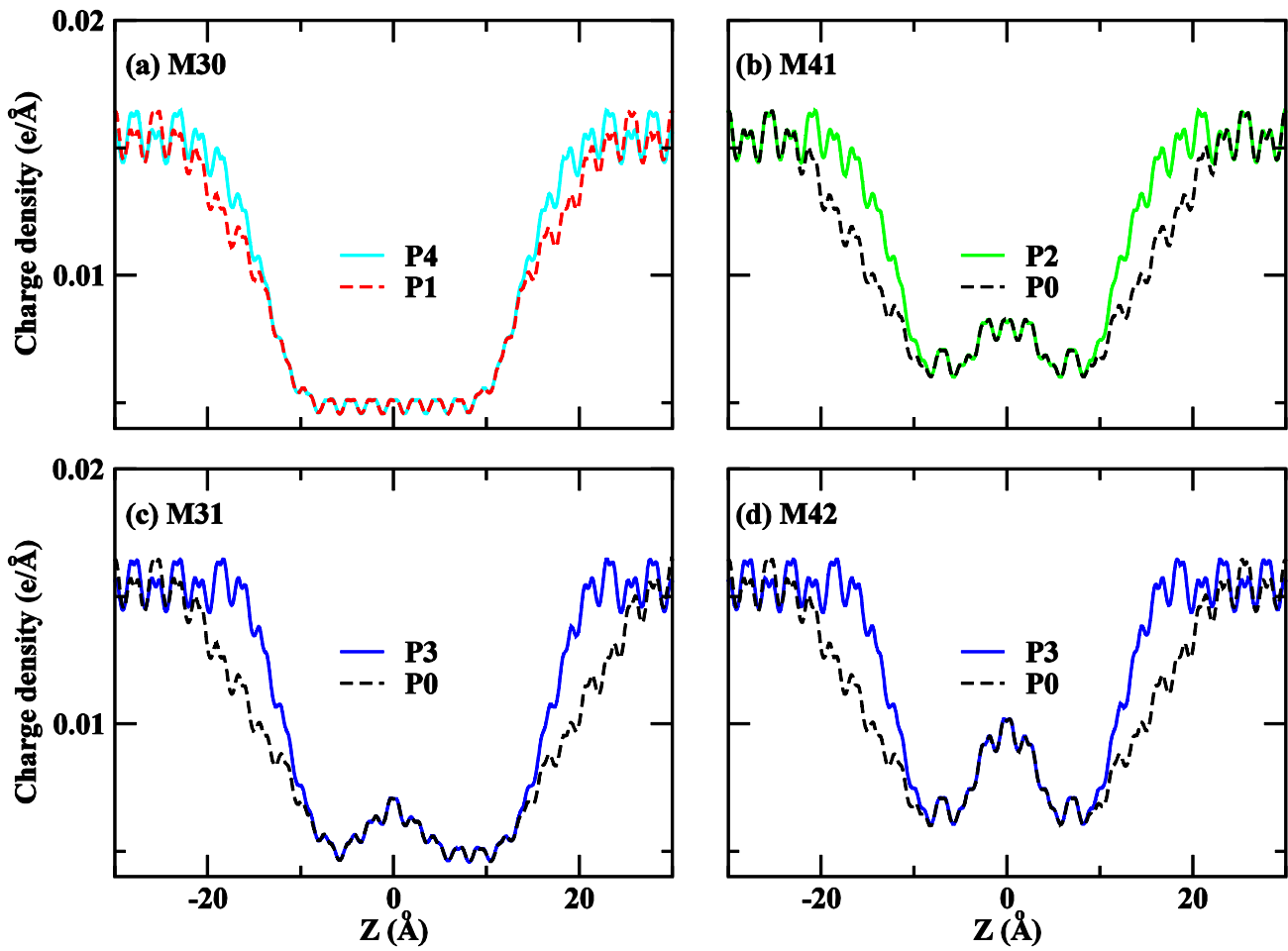


Fig. S3 Plane-averaged charge density for (a) S_{M30P4} , S_{M30P1} ; (b) S_{M41P2} , S_{M41P0} ; (c) S_{M31P3} , S_{M31P0} ; (d) S_{M42P3} , S_{M42P0} . The colors for each model correlate with those in Fig. 1.

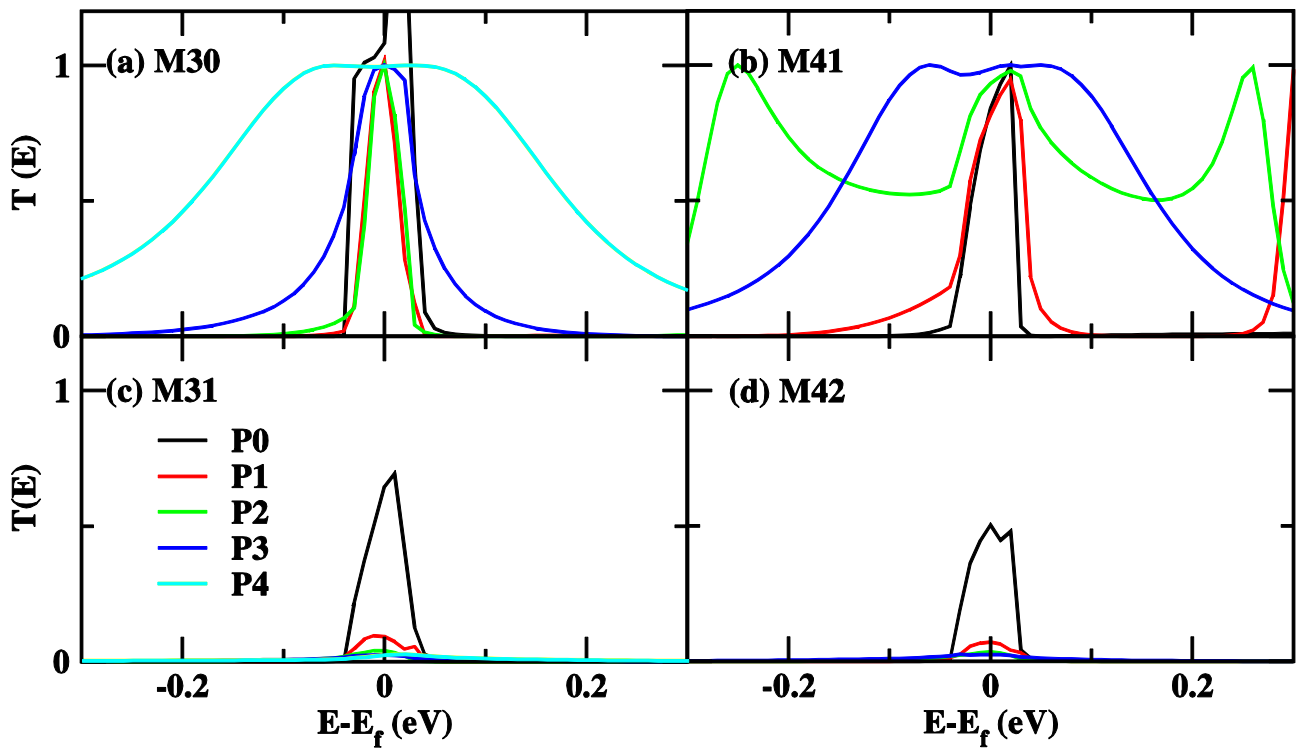


Fig. S4 Position dependent transmission spectra of (a) S_{M30Pq} ; (b) S_{M41Pq} ; (c) S_{M31Pq} , and (d) S_{M42Pq} . ZGNR with 11 zigzag chains (ZGNR-11) serves as the electrode.

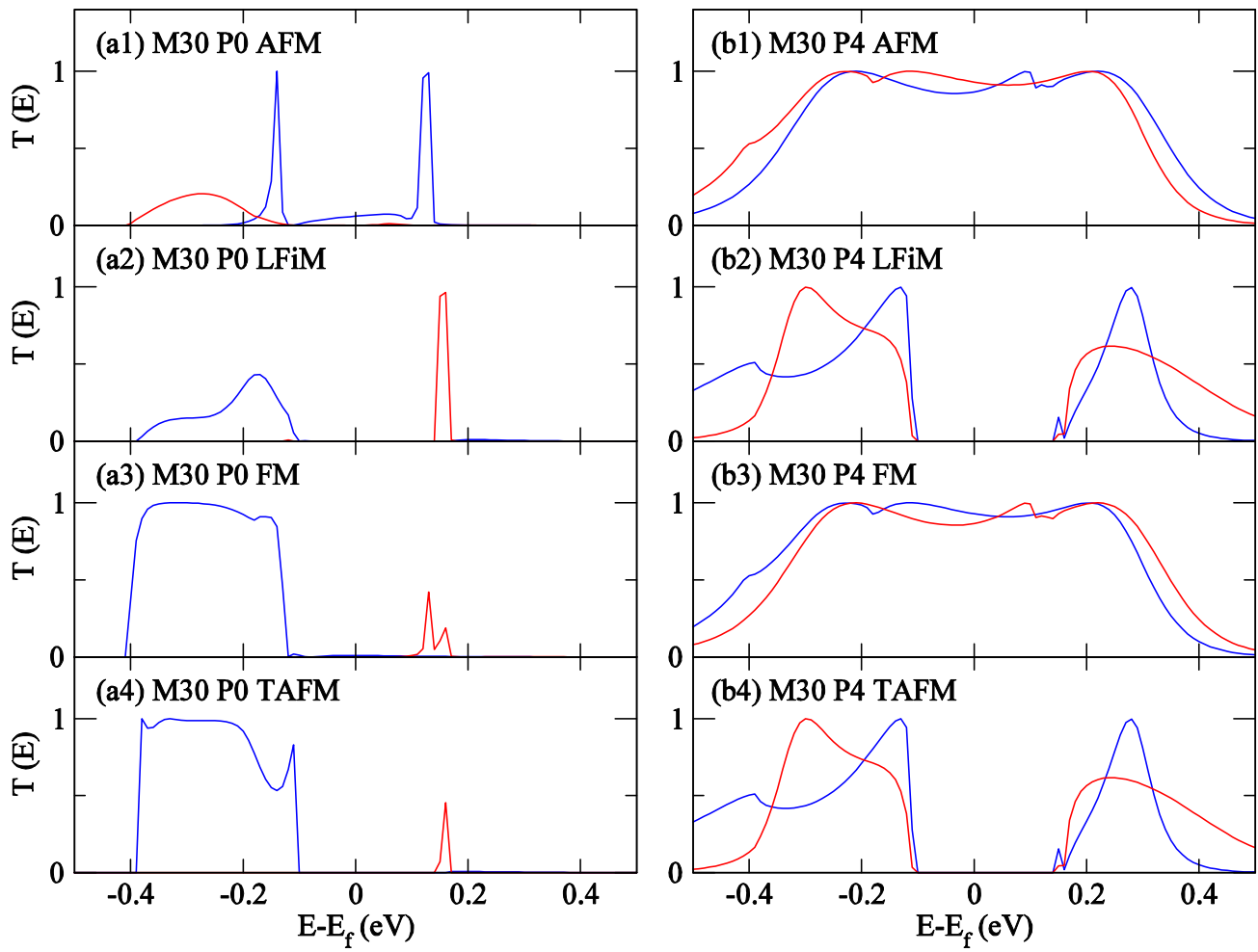


Fig. S5 Transmission for M30 at two positions: (a1)-(a4) S_{M30P0} ; (b1)-(b4) S_{M30P4} . Antiferromagnetic (AFM), longitudinal-ferrimagnetic (LFiM), ferromagnetic (FM), and trans-antiferromagnetic (TAFM) configurations are considered at each position, following ref [1].

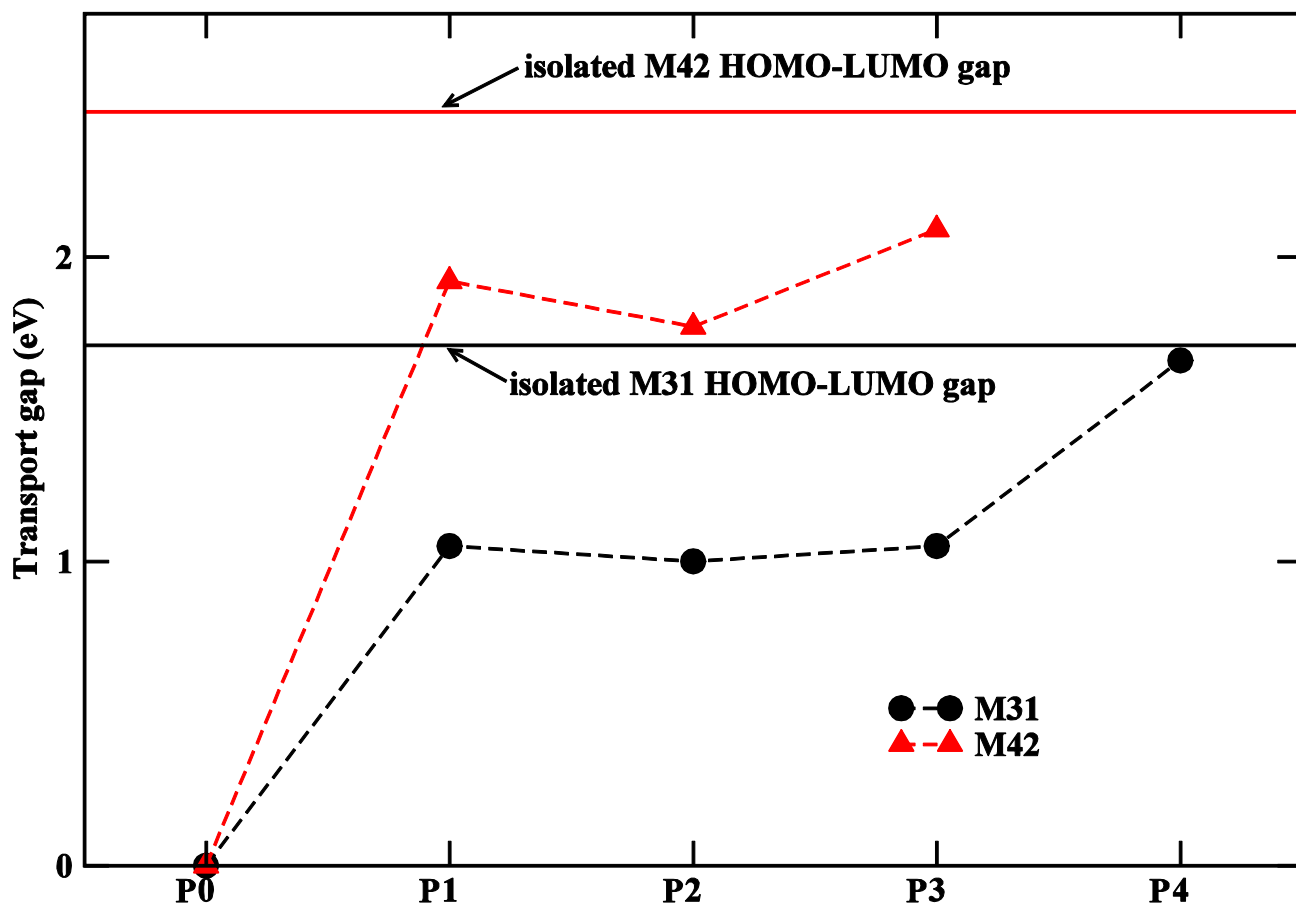


Fig. S6 Transport gap for M31 and M42 at different positions. The straight lines are guides for the eye.

[1] E. C. Girão, E. Cruz-Silva, L. Liang, A. G. Souza Filho and V. Meunier, *Phys. Rev. B*, 2012, **85**, 235431.