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I-V Characteristics of Thiophene Functionalized Metalla-Bis(Dicarbollide)

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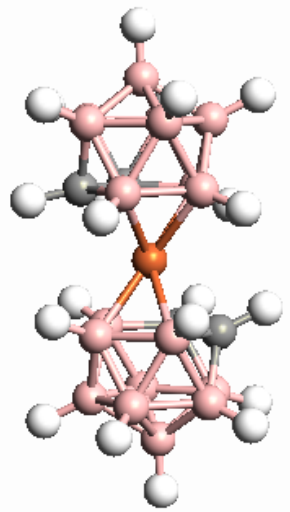
What is thiophene functionalized metalla-bis(dicarbollide)?

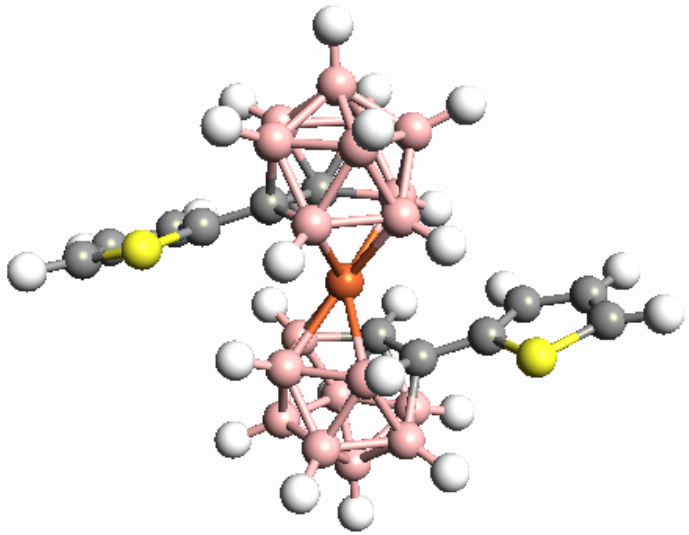
Central transition metal atom(Fe(III))

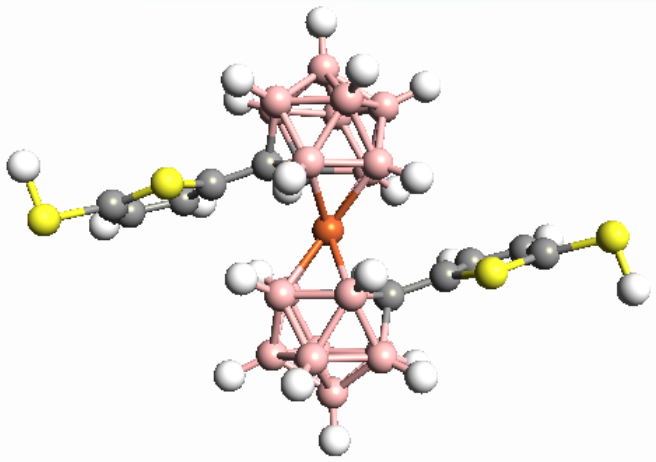
Carborane cages

Thiophene rings

Linking atoms(S)



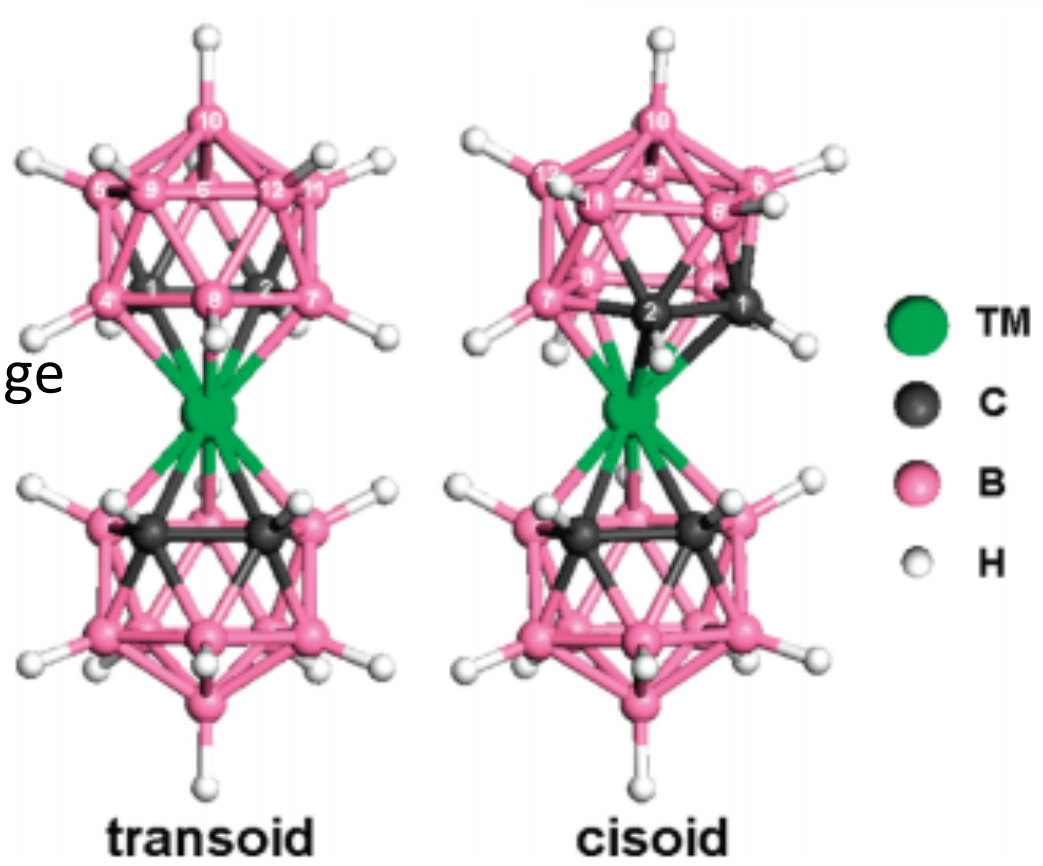




Previous Research

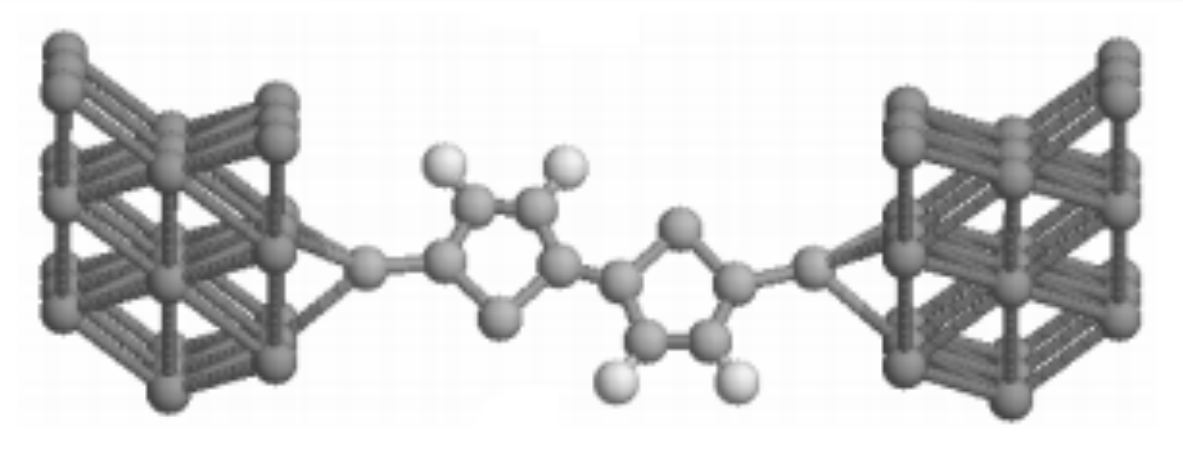
Dicarbollide

- Low Rotational Barrier
- Magnetic Information Storage
- Molecular Rotor



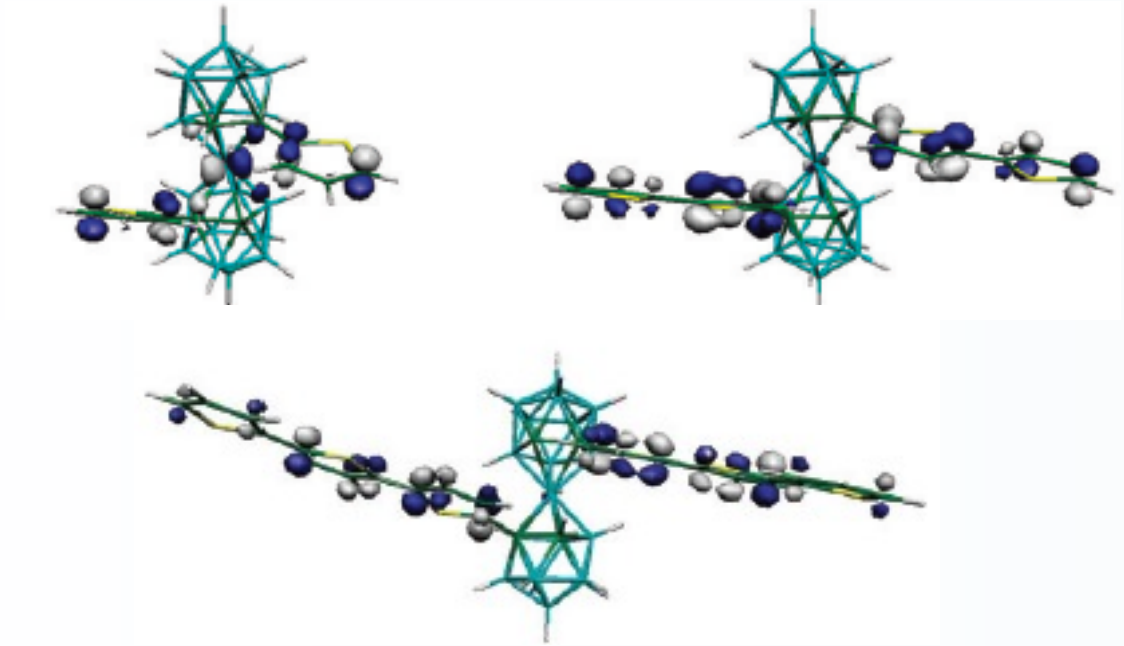
Thiophene Rings

- Many Possible Torsional Angles
- Each Exhibits Different Energy Gap
- Variable Conductance
- Applicable for Molecular Switch



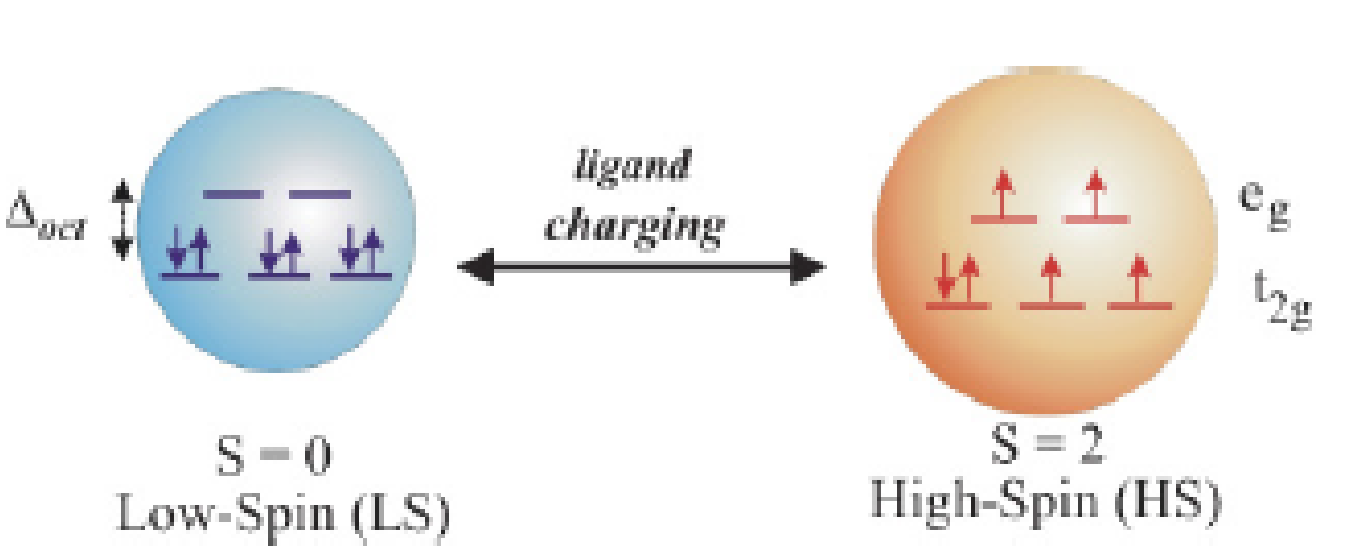
Thiophene Functionalized Co-bis(dicarbollide)

- Exhibits High Stability
- Experimentally Synthesized
- Increased conductance with higher number of thiophene rings



Spin Cross-over Systems

- Spin State Manipulated
- Transition Reversible



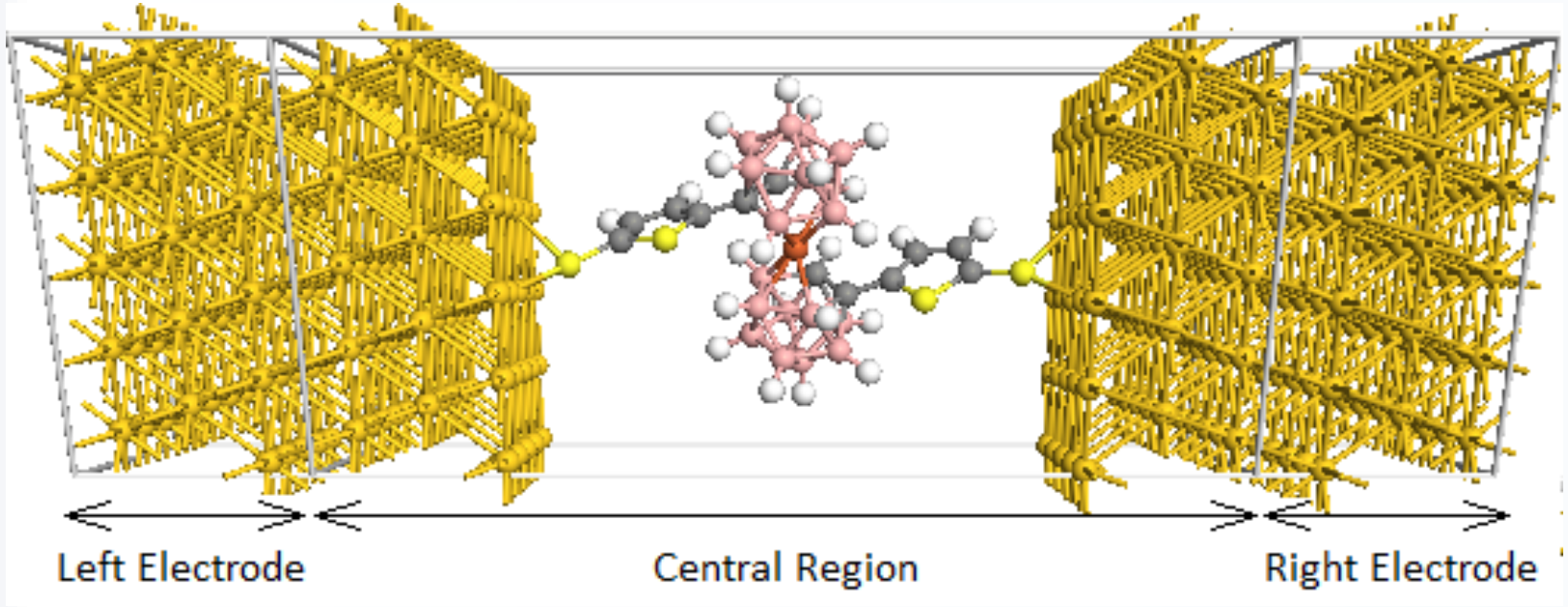
Methods

Gaussian

- Assemble Molecule
- Geometrically Optimize
- Set Spin State

Atomistix

- Create Device
- Set Initial Spin State
- Perform Electron Transport Calculations



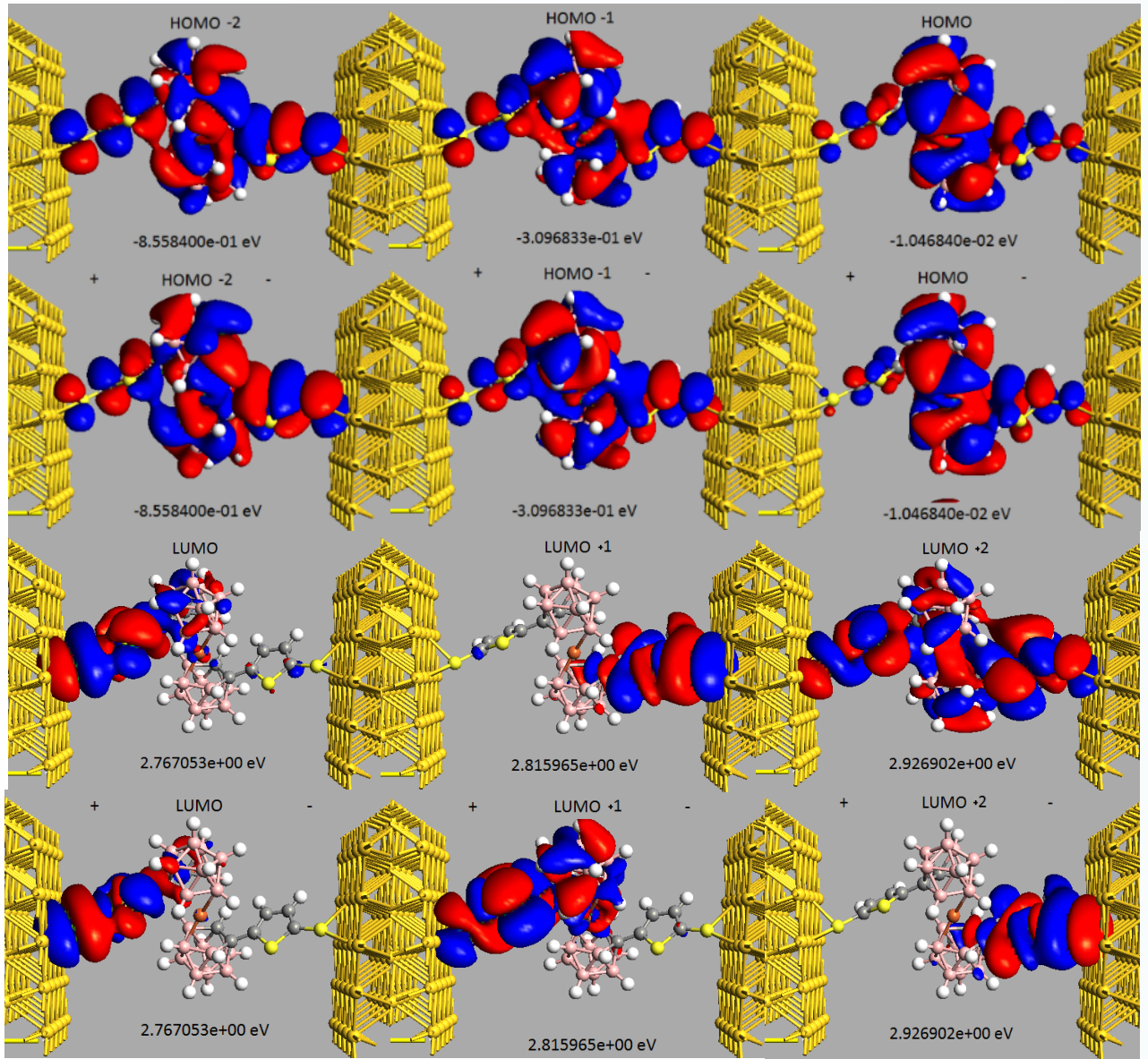
Projected Orbitals

0.0V

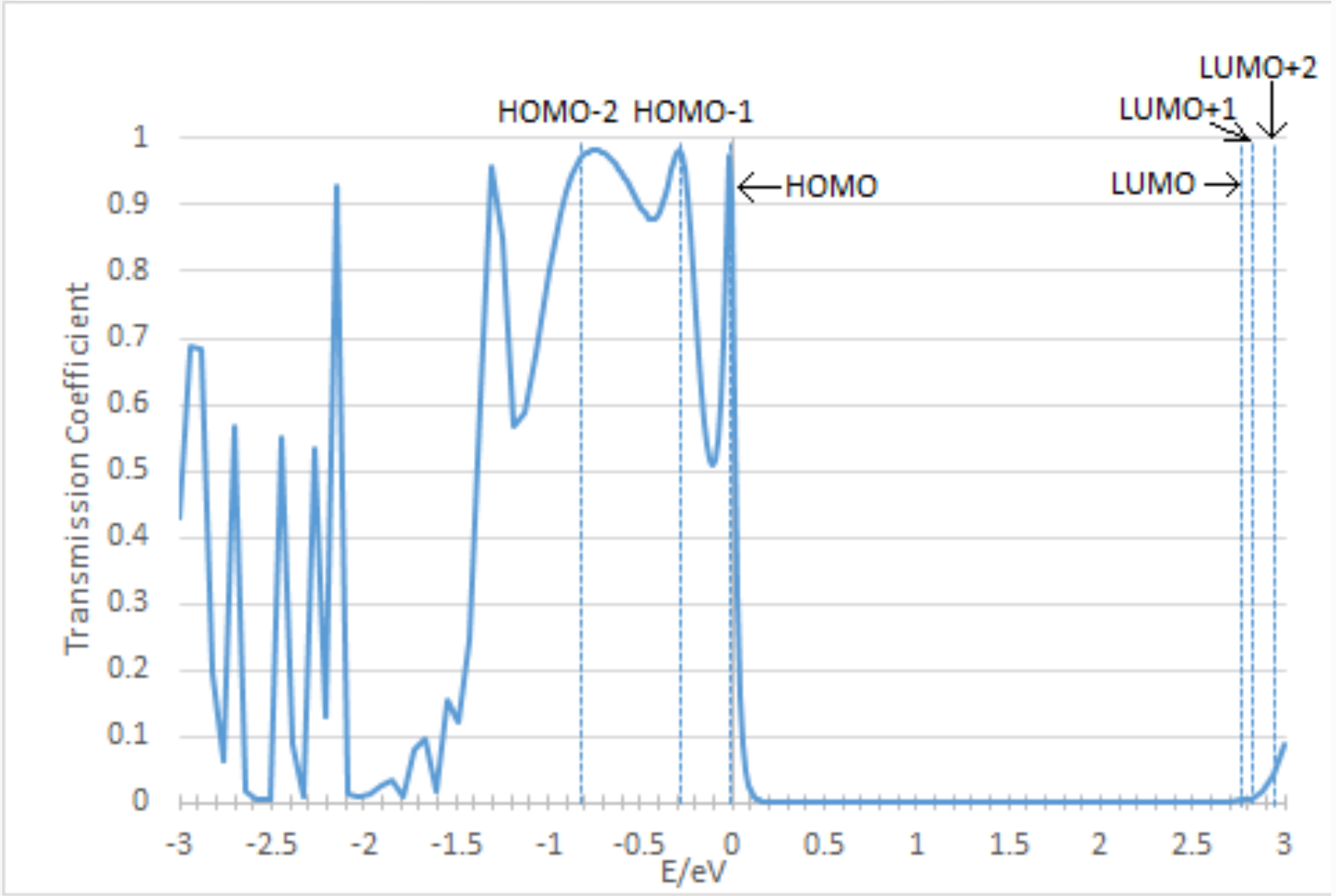
1.0V

0.0V

1.0V



Transmission Spectrum 0.0V



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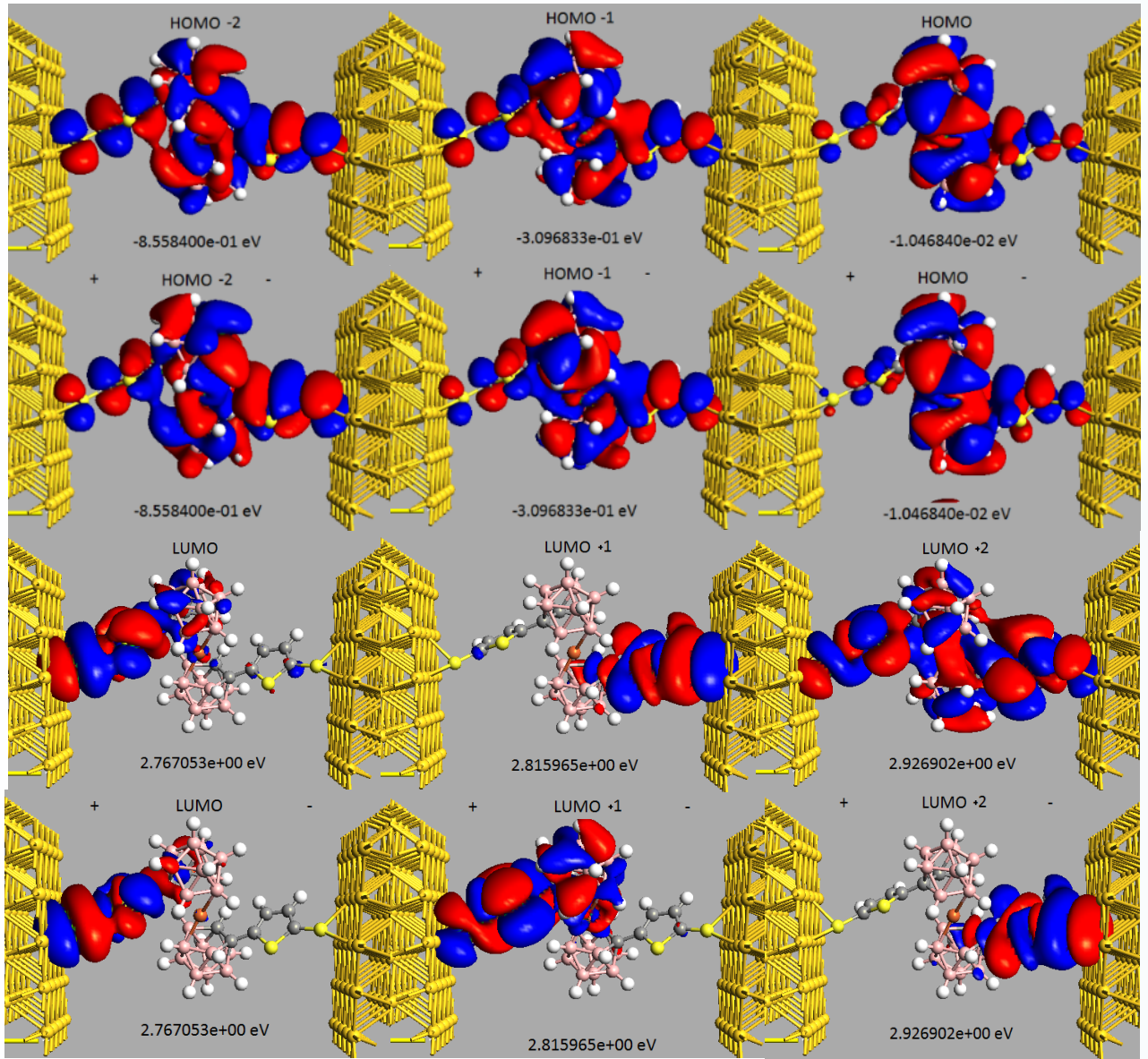
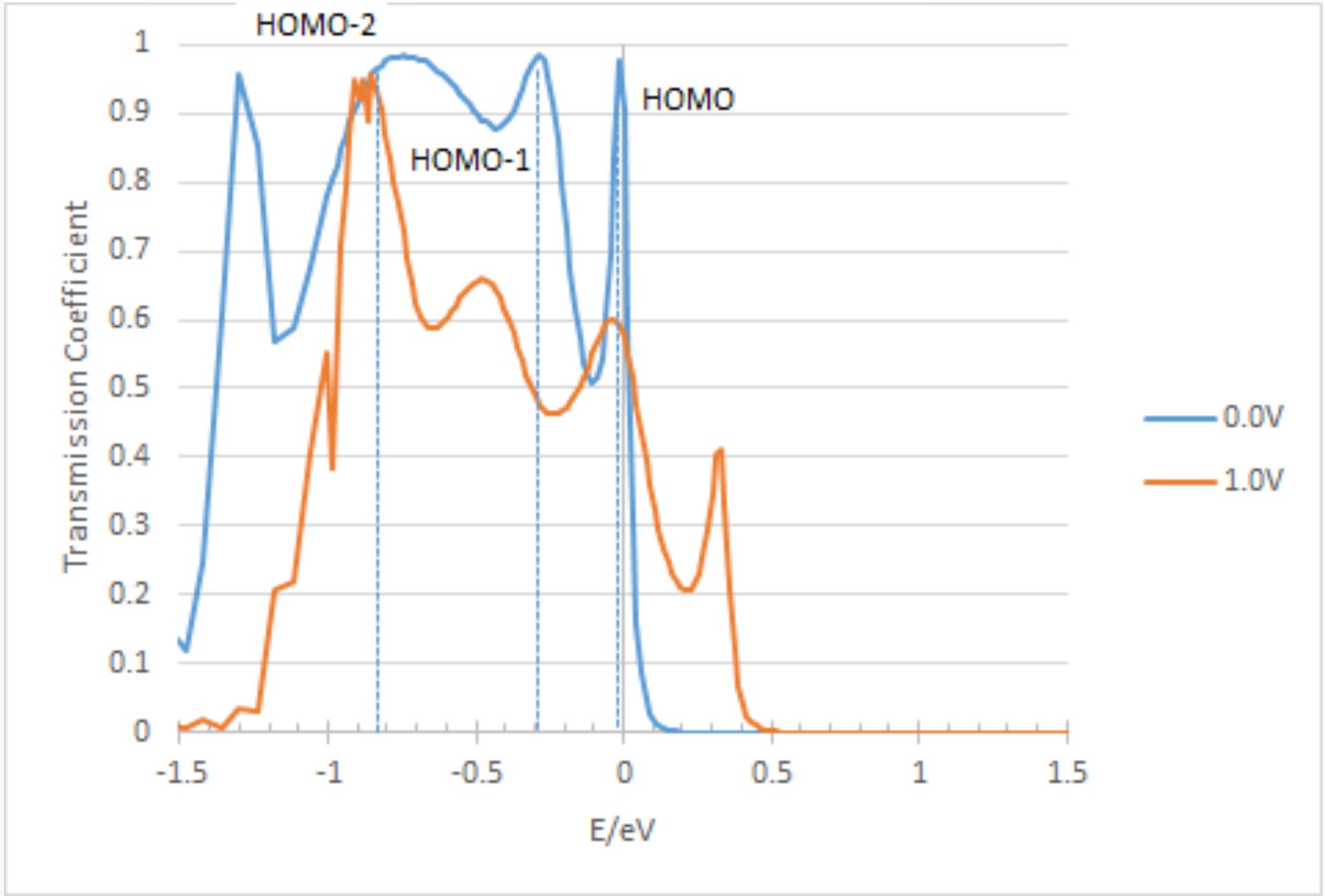
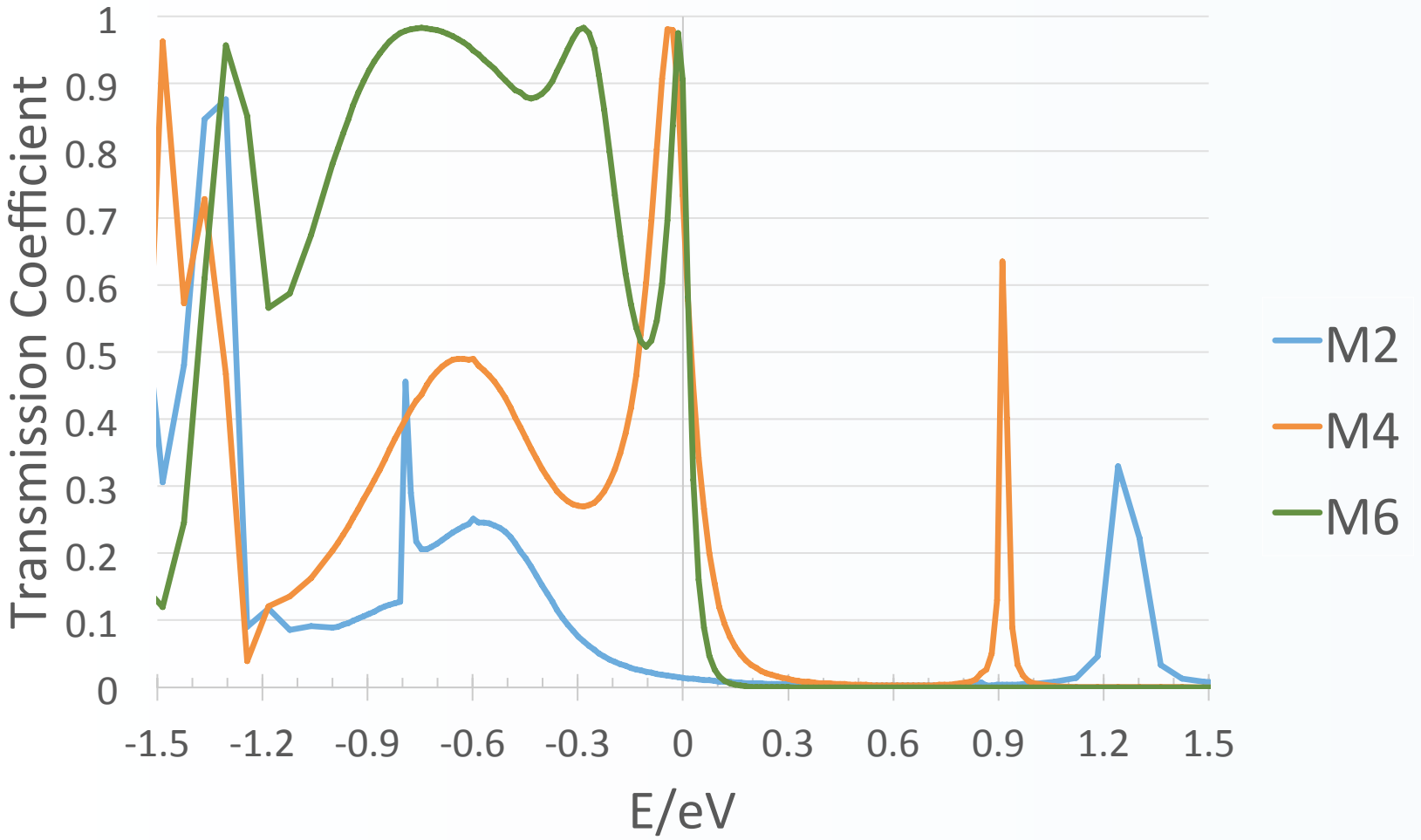


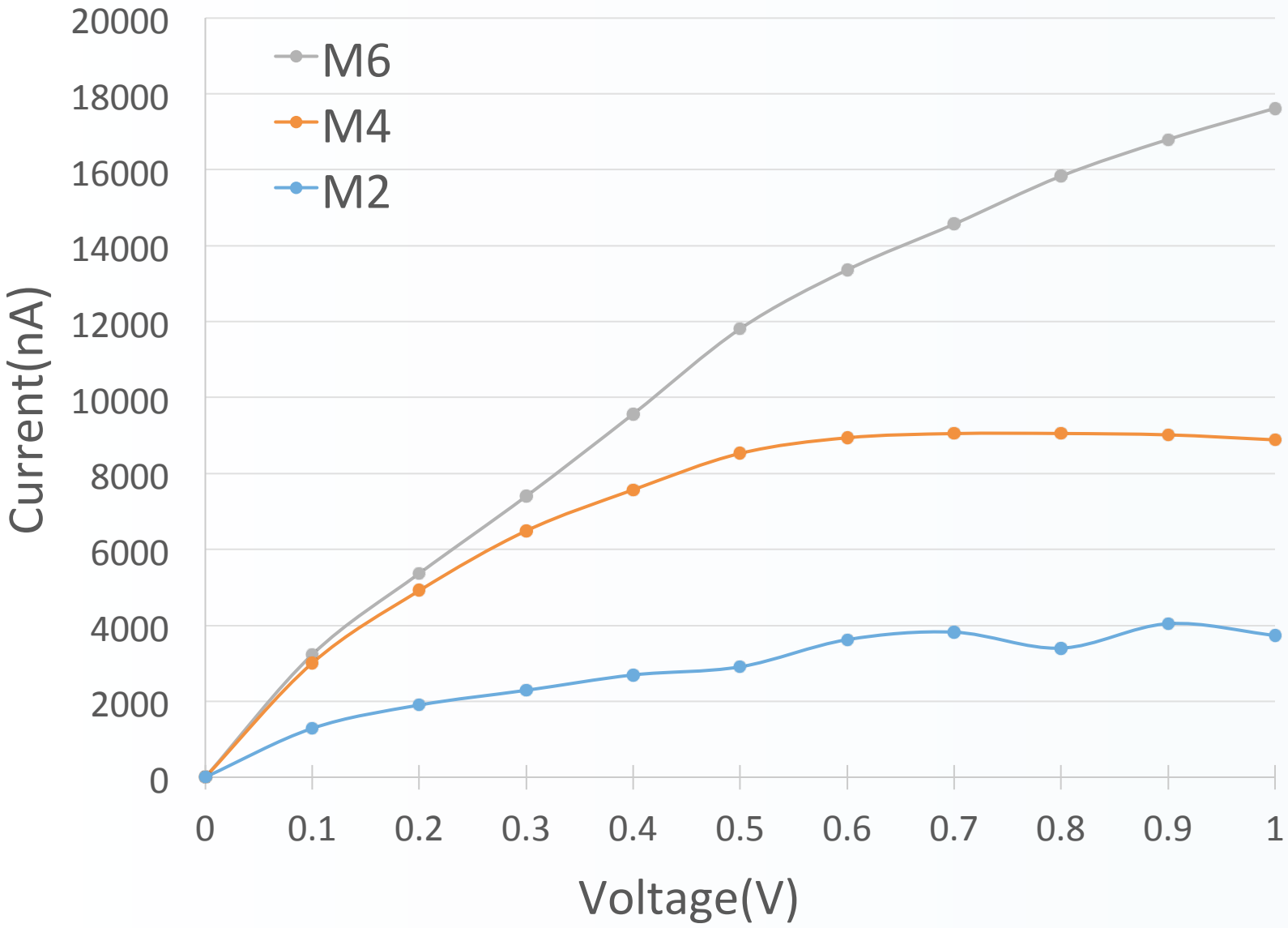
Transmission Spectrum 1.0V



Transmission Spectrum Comparison Between Spin States



I-V Characteristics

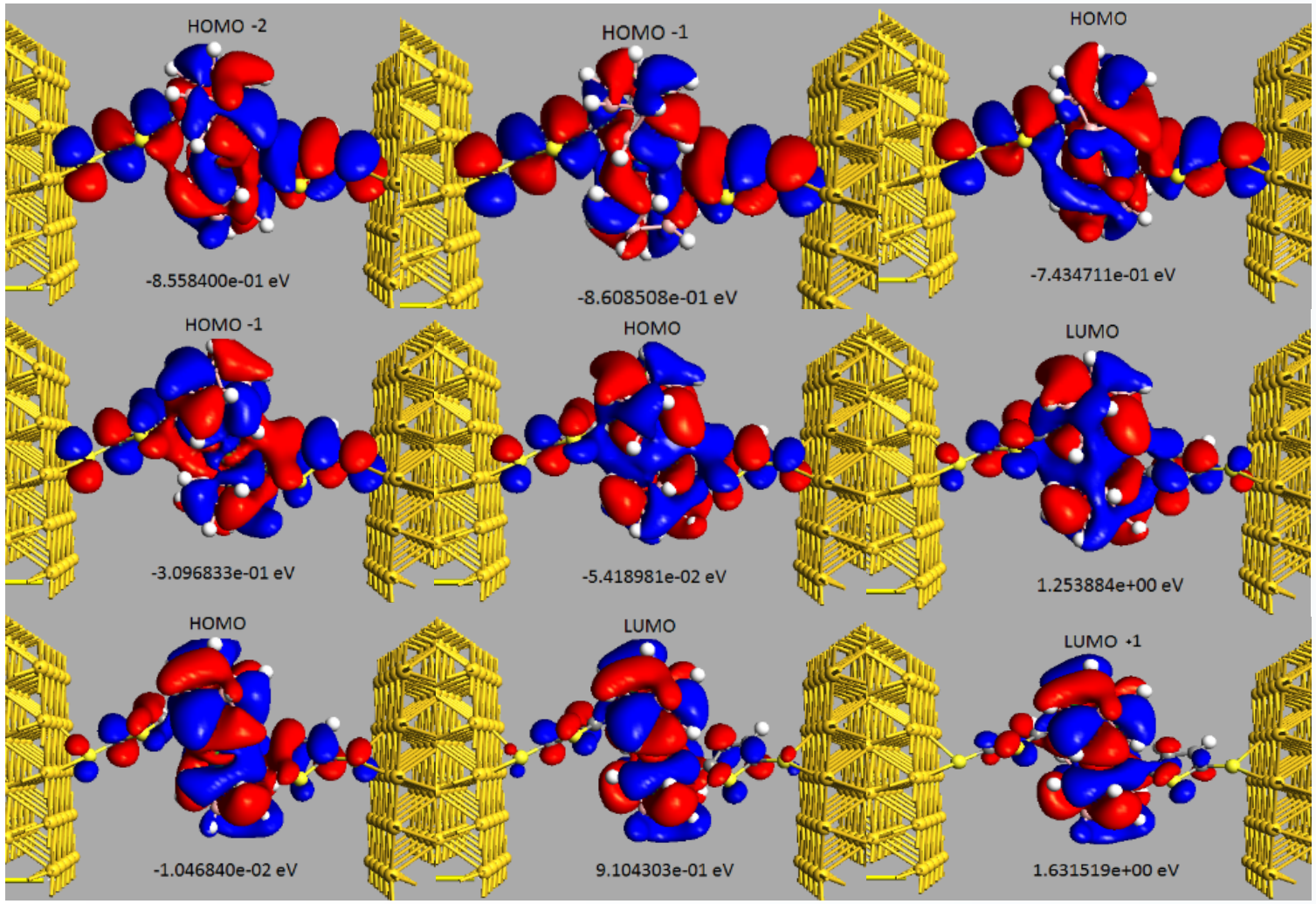


Orbital Populations

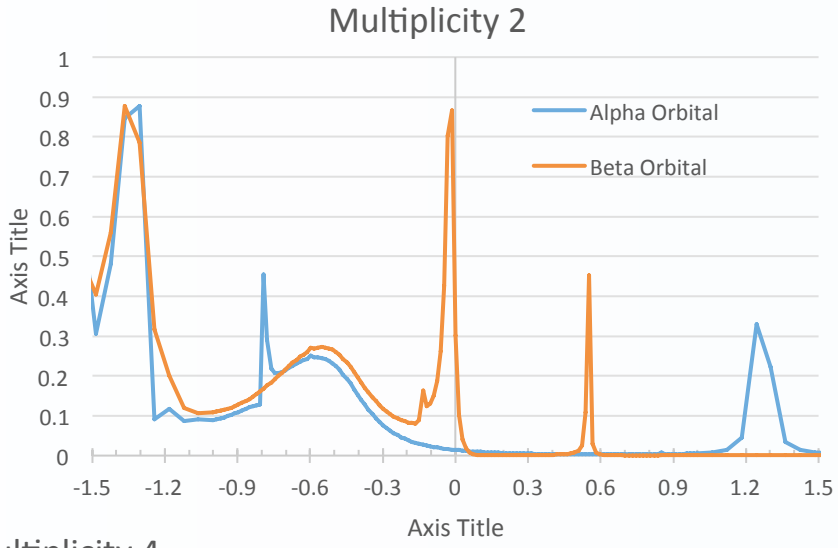
	Spin Up			Spin Down			
	Orbital #	Energy(eV)	# of electrons	Orbital #	Energy(eV)	# of electrons	Electron population
Multiplicty: 2	77	-1.085387e+00	1.000000e+00	77	-7.442891e-01	1.000000e+00	
	78	-9.647852e-01	1.000000e+00	78	-1.437669e-01	9.961704e-01	
	79	-7.962475e-01	1.000000e+00	79	-2.405240e-02	7.171539e-01	
	80	-7.434711e-01	1.000000e+00	80	5.460652e-01	6.706862e-10	
	81	1.253884e+00	8.623787e-22	81	1.797860e+00	6.270591e-31	
	82	1.631519e+00	3.905830e-28	82	2.092719e+00	6.980905e-36	
	83	2.820910e+00	3.720076e-44	83	2.823848e+00	3.720076e-44	
	84	2.826026e+00	3.720076e-44	84	2.829435e+00	3.720076e-44	
Multiplicity: 4	77	-1.405357e+00	1.000000e+00	77	-8.559476e-01	1.000000e+00	
	78	-1.284445e+00	1.000000e+00	78	-5.189634e-02	8.815758e-01	
	79	-1.125772e+00	1.000000e+00	79	3.408515e-01	1.879111e-06	
	80	-8.608508e-01	1.000000e+00	80	7.488131e-01	2.633346e-13	
	81	-5.418981e-02	8.905287e-01	81	1.227755e+00	2.369483e-21	
	82	9.104303e-01	5.075306e-16	82	1.676005e+00	6.988468e-29	
	83	2.810562e+00	3.720076e-44	83	2.804492e+00	3.720076e-44	
	84	2.815739e+00	3.720076e-44	84	2.809489e+00	3.720076e-44	
Multiplicity: 6	77	-1.523641e+00	1.000000e+00	77	-7.943262e-01	1.000000e+00	
	78	-1.349848e+00	1.000000e+00	78	9.129902e-02	2.842637e-02	
	79	-1.221091e+00	1.000000e+00	79	1.084801e-01	1.482953e-02	
	80	-8.558400e-01	1.000000e+00	80	5.185879e-01	1.941408e-09	
	81	-3.096833e-01	9.999937e-01	81	8.629067e-01	3.190226e-15	
	82	-1.046840e-02	5.998728e-01	82	1.090908e+00	4.716009e-19	
	83	2.767053e+00	3.720076e-44	83	2.768215e+00	3.720076e-44	
	84	2.815965e+00	3.720076e-44	84	2.811989e+00	3.720076e-44	

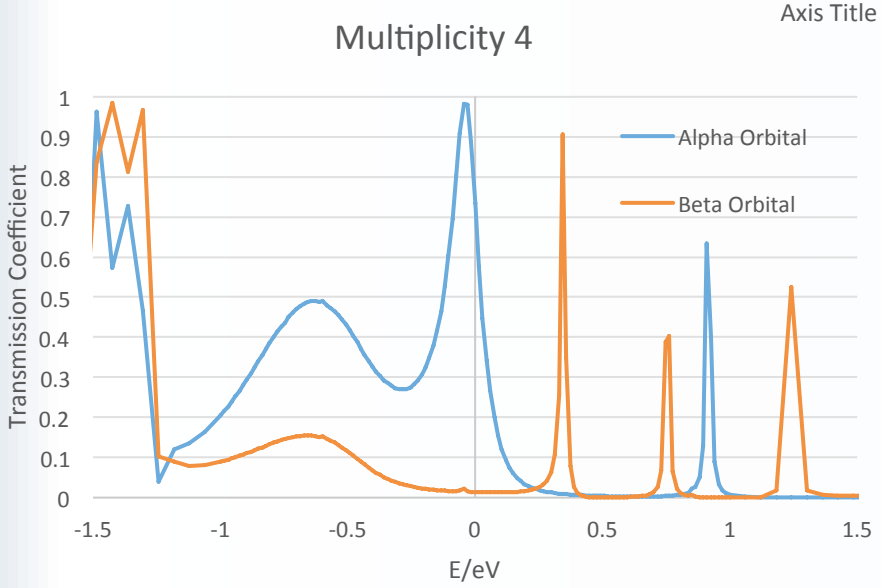
Orbital Comparison

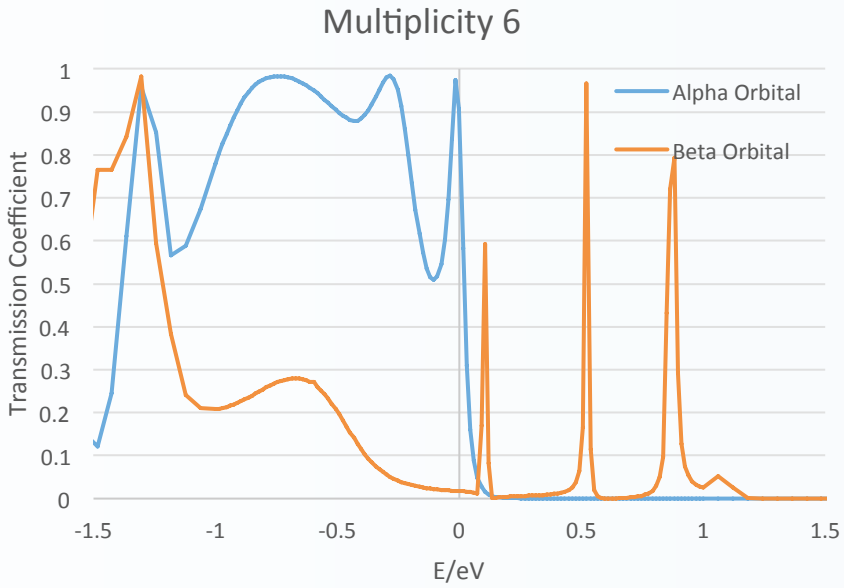
Multiplicity: 6 **Multiplicity: 4** **Multiplicity: 2**



Transmission Spectra of Alpha and Beta Orbitals







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References

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