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

Supplementary Information

Spin-polarized transport properties in some transition metal dithiolene complexes

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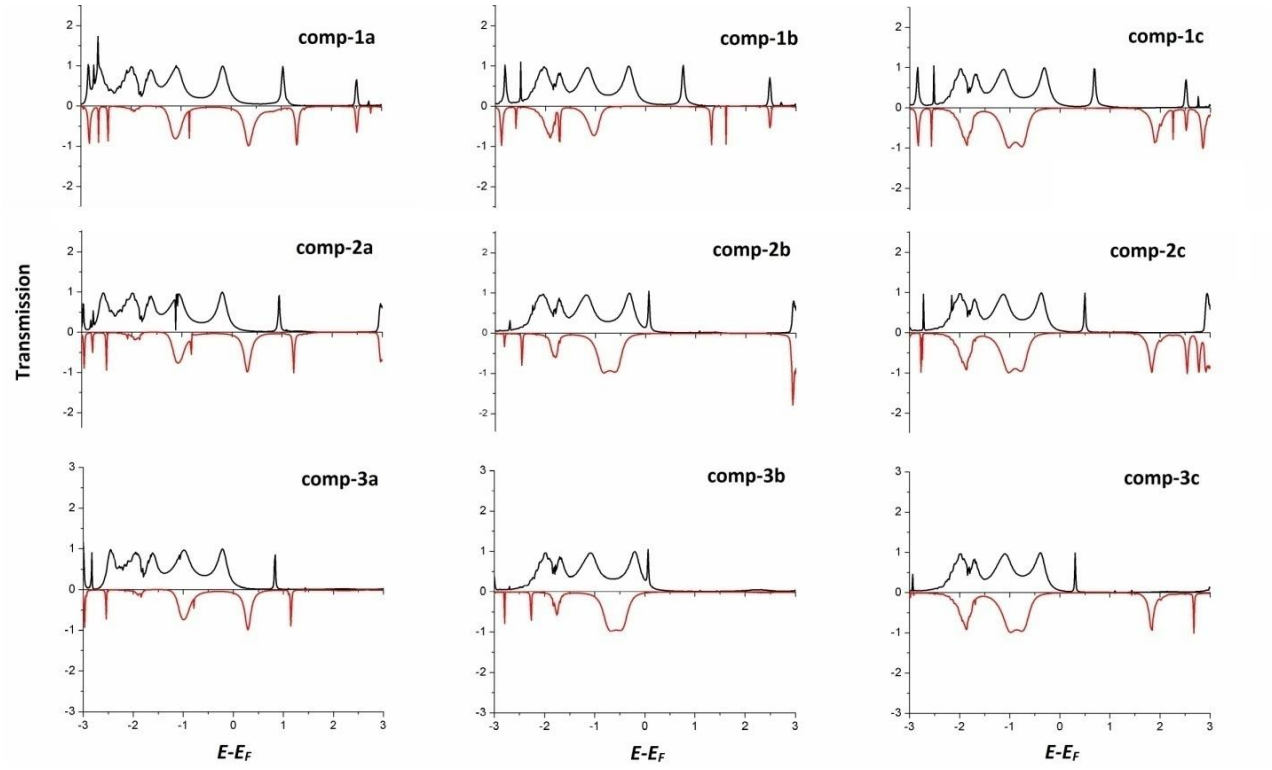
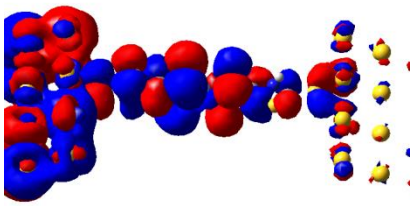
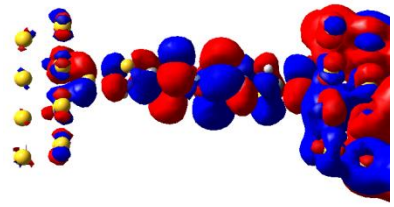


Figure S1 The spin-resolved transmission spectra at zero bias of complexes **1a-1c, 2a-2c** and **3a-3c**.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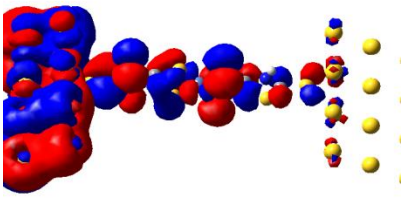	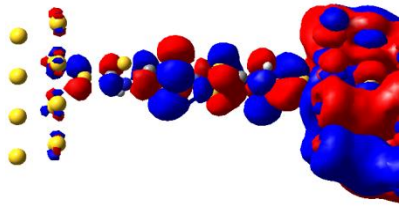
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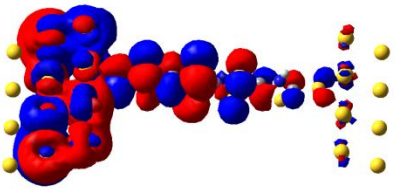
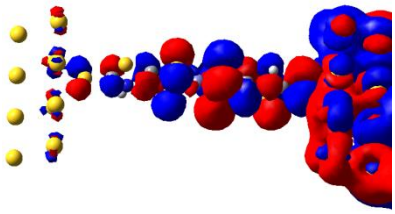
Compound **2a**	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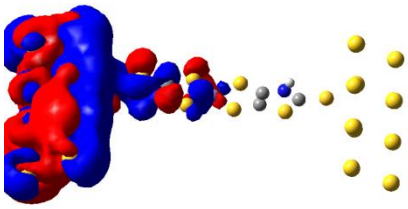	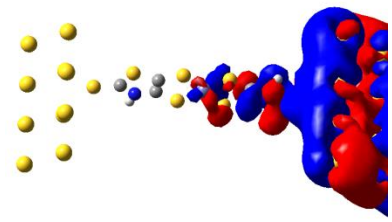
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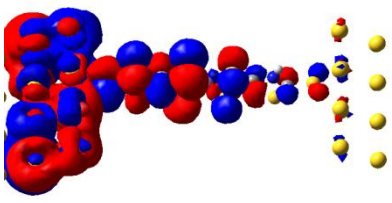
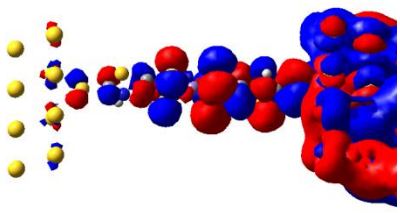
Compound **2b**	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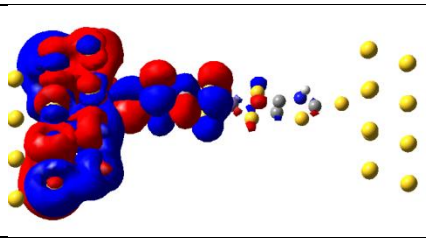	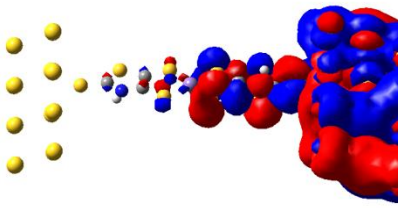
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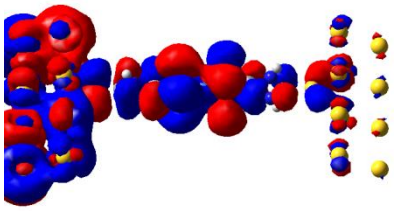
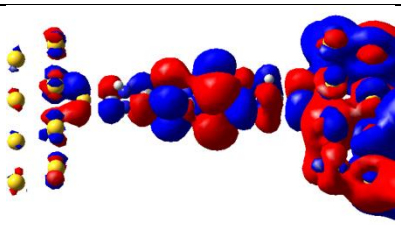
Compound **2c**	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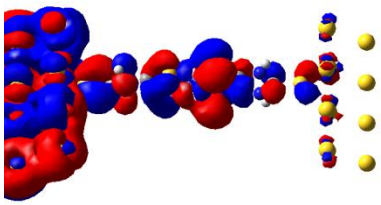	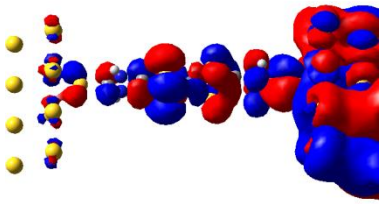
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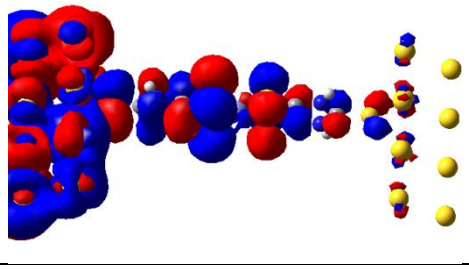
Compound **3a**	



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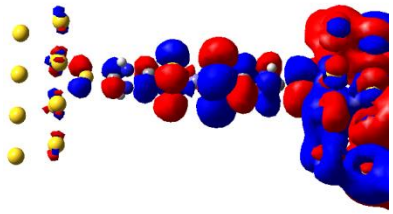

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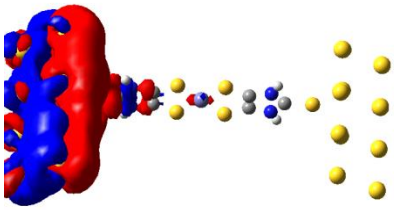

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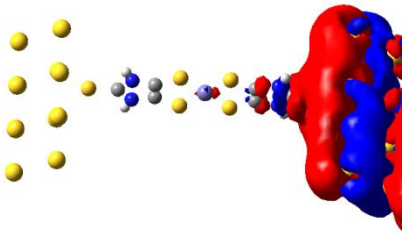

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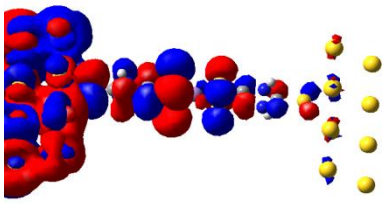
Compound **3b**



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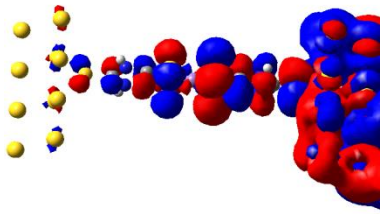

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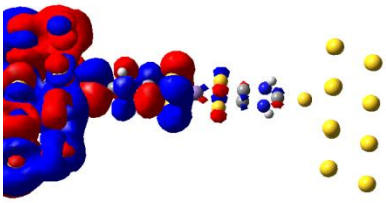

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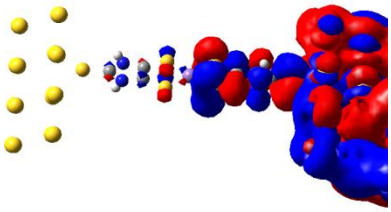

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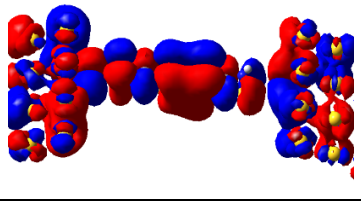
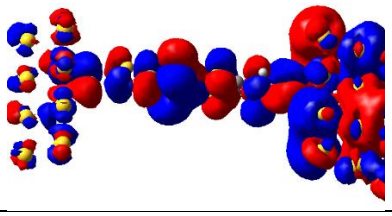
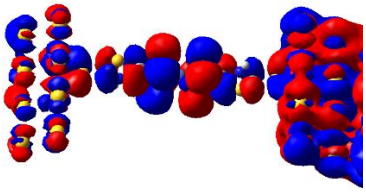
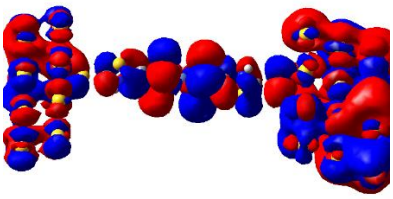
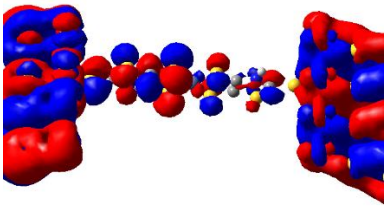
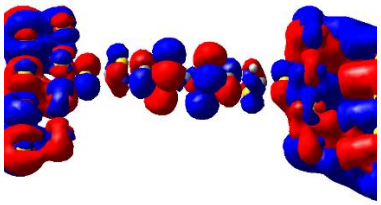
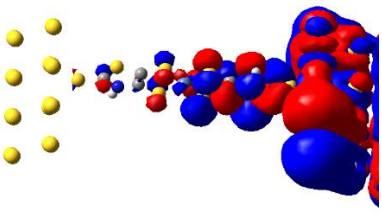
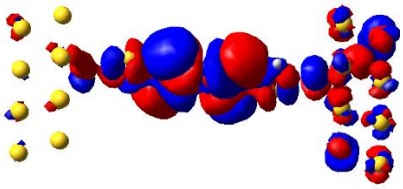
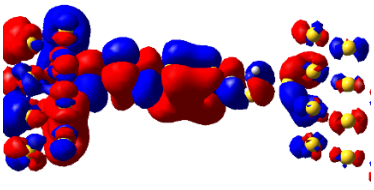
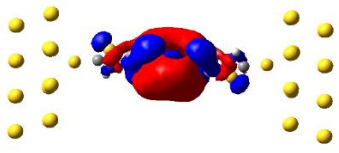
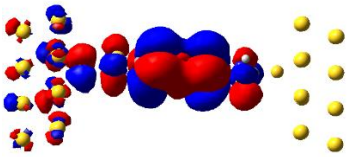
Compound **3c**

Figure S2: The first eigenchannels at Fermi level for complexes **2a**-**2c** and **3a**-**3c**

		
α-475	**α-479**	**α-482**
		
α-488	**α-495**	**α-497**
		
α-506	**α-509**	

α-spin MPSH orbitals of **2a**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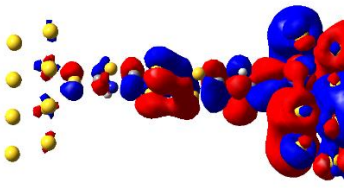	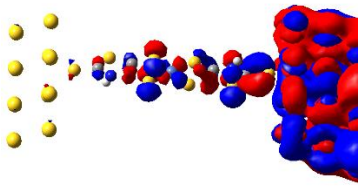	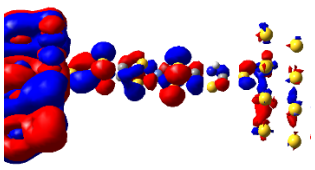
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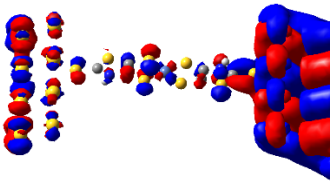	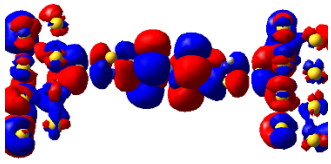	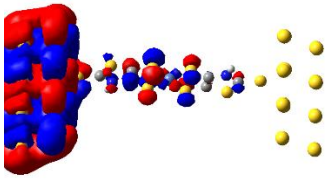
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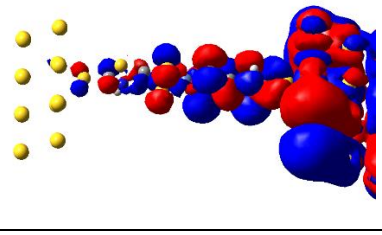
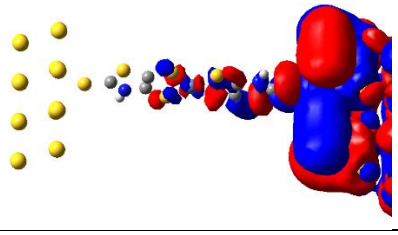
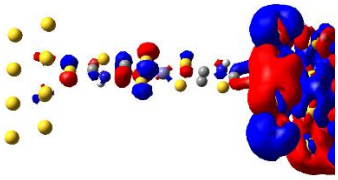
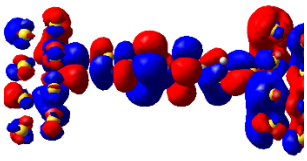
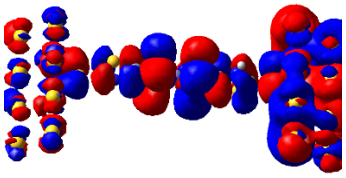
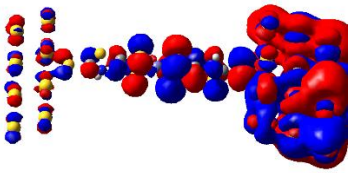
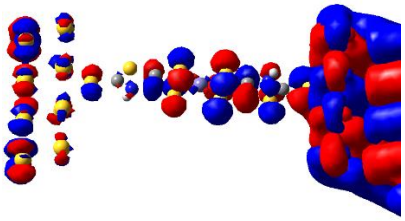
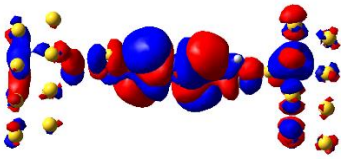
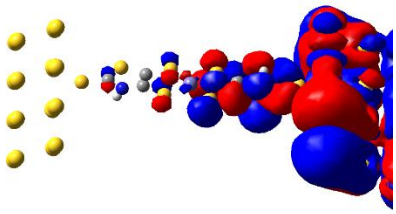
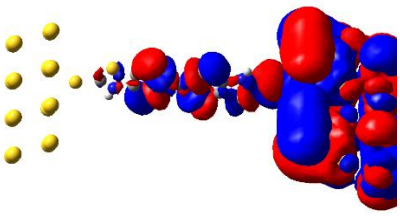
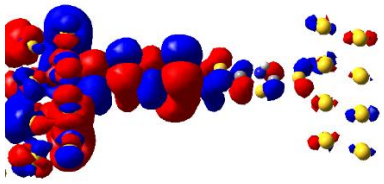
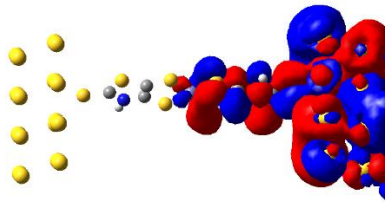
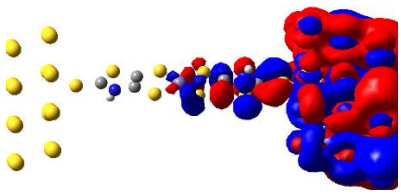
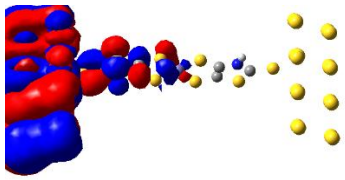
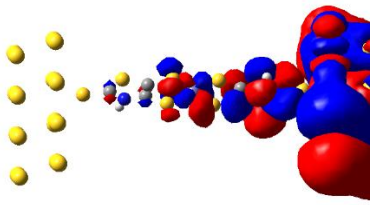
		
β-506	**β-507**	

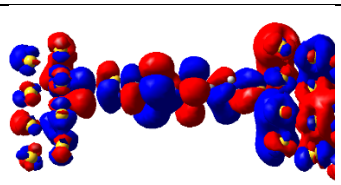
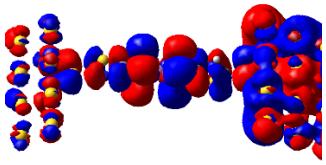
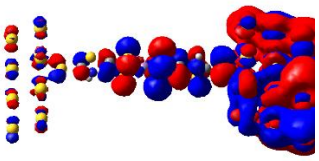
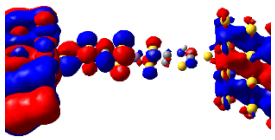
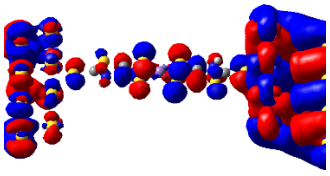
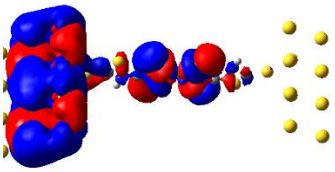
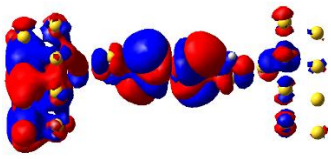
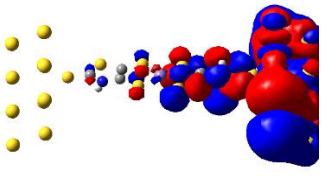
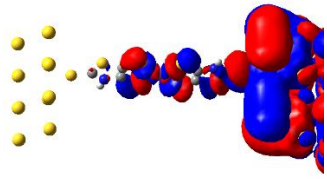
β-spin MPSH orbitals of **2a**

		
α-477	**α-479**	**α-482**
		
α-488	**α-495**	**α- 497**
		
α- 502	**α-507**	**α-508**

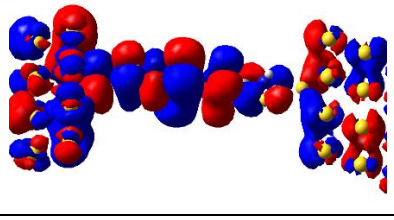
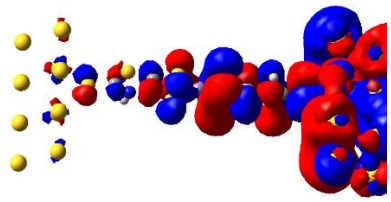
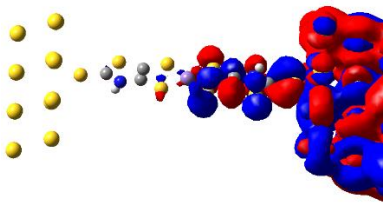
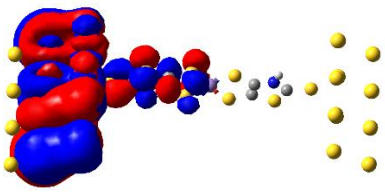
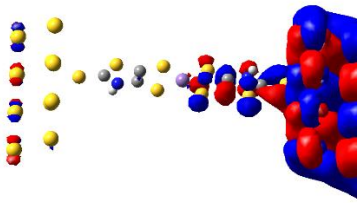
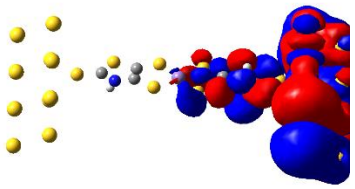
α-spin MPSH orbitals of **2b**

		
β-473	**β-478**	**β-484**
		
β-491	**β-503**	

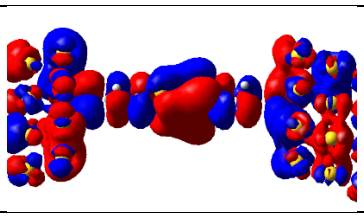
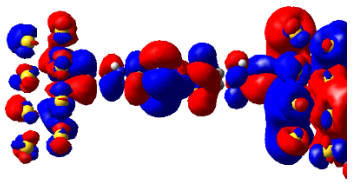
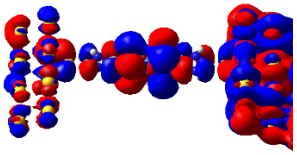
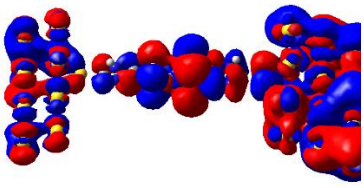
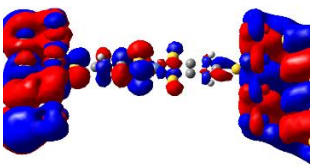
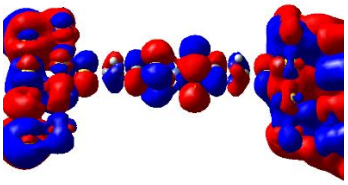
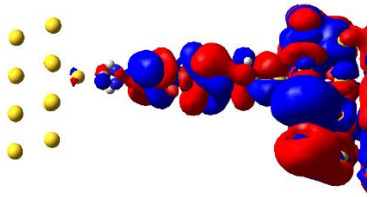
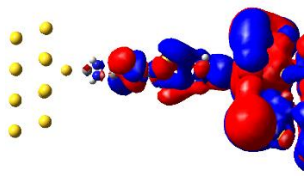
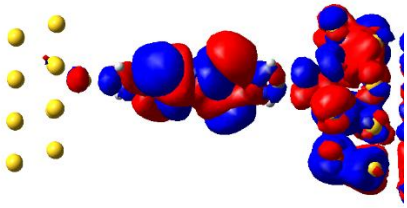
β-spin MPSH orbitals of **2b**

		
α-479	**α-482**	**α- 488**
		
α-495	**α-497**	**α-501**
		
α-502	**α-507**	**α-508**

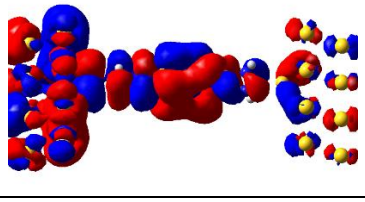
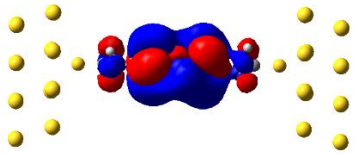
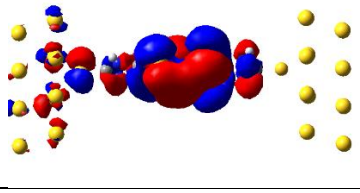
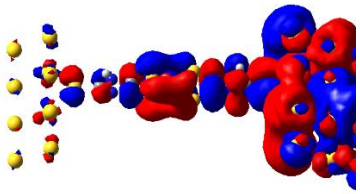
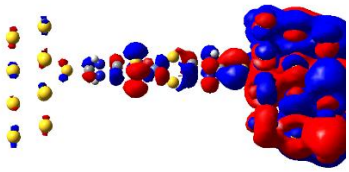
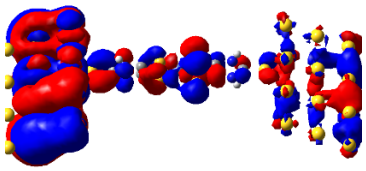
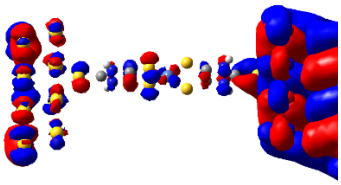
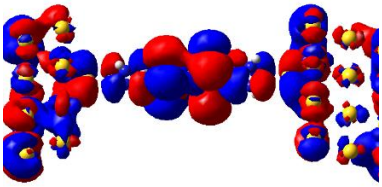
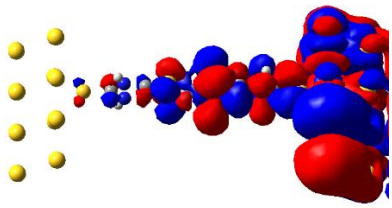
α-spin MPSH orbitals of **2c**

		
β-472	**β-478**	**β-484**
		
β-490	**β-492**	**β-502**

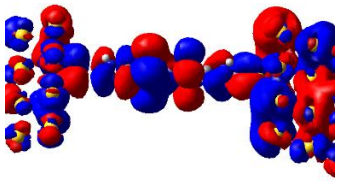
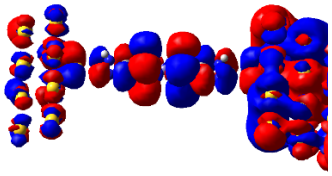
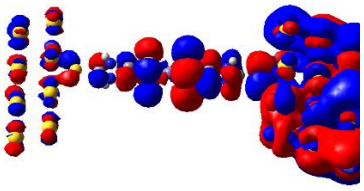
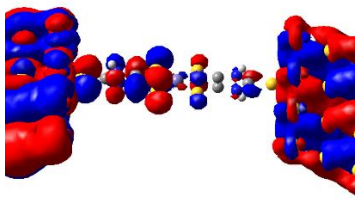
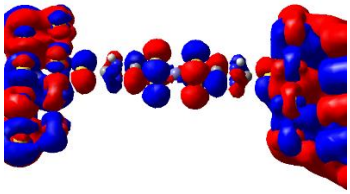
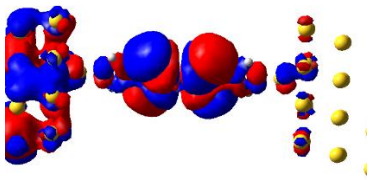
β-spin MPSH orbitals of **2c**

		
α-475	**α-479**	**α-482**
		
α-488	**α-495**	**α-497**
		
α-506	**α-507**	**α-508**

α-spin MPSH orbitals of **3a**

		
β-473	**β-474**	**β-475**
		
β-481	**β-486**	**β-493**
		
β-495	**β-498**	**β-506**

β-spin MPSH orbitals of **3a**

		
α-479	**α-482**	**α-488**
		
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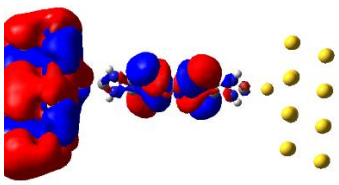
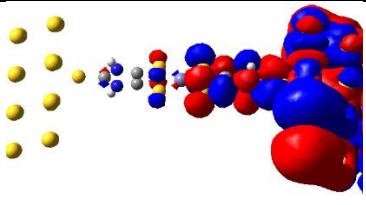
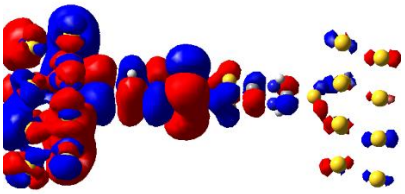
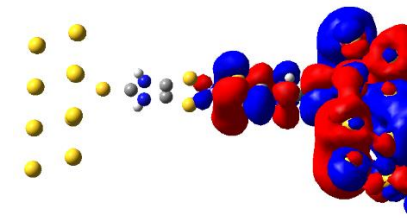
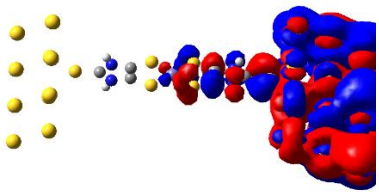
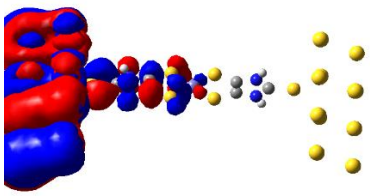
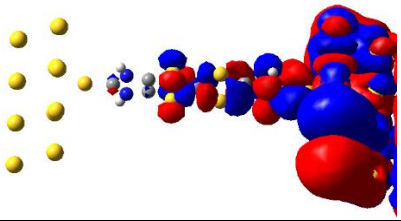
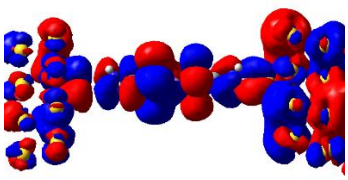
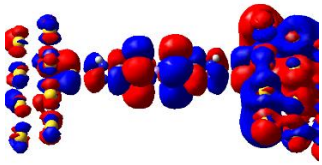
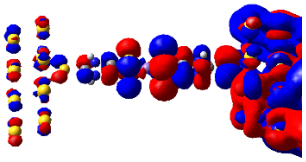
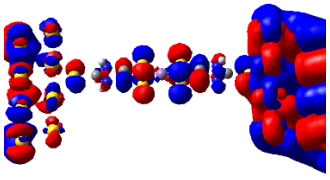
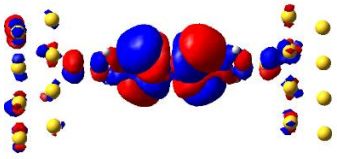
		
α-502	**α-507**	

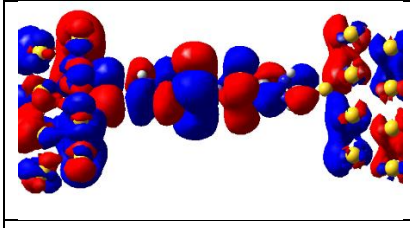
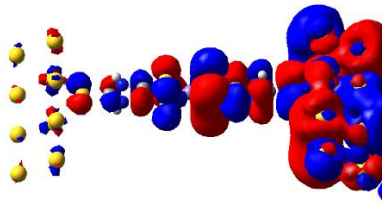
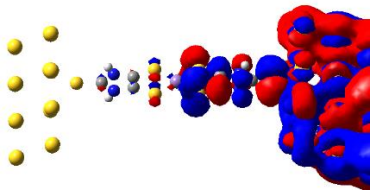
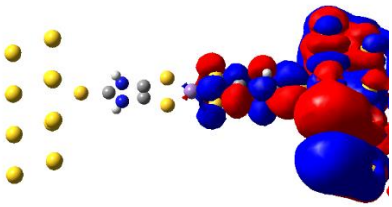
α-spin MPSH orbitals of **3b**

		
β-473	**β-479**	**β-485**
		
β-491	**β-503**	

β-spin MPSH orbitals of **3b**

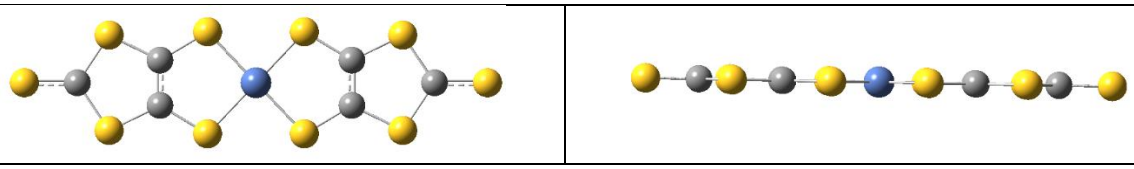
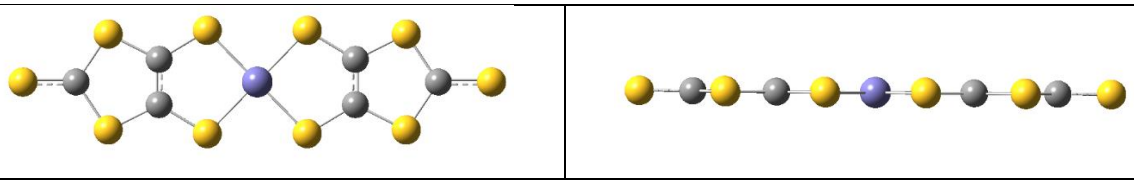
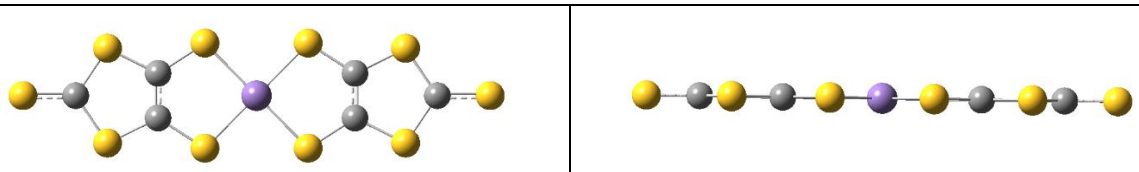
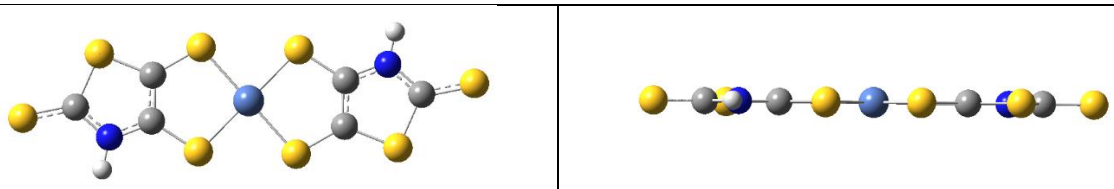
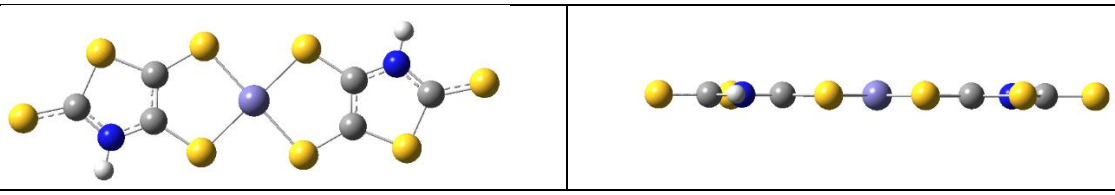
		
α-479	**α-482**	**α-488**
		
α-495	**α-497**	**α-499**

α-spin MPSH orbitals of **3c**

		
β-472	**β-478**	**β-484**
		
β-491	**β-501**	

β-spin MPSH orbitals of **3c**

Figure S3 The partial distribution of MPSH orbitals of complexes **2a-2c** and **3a-3c**

1a

1b

1c

2a

2b

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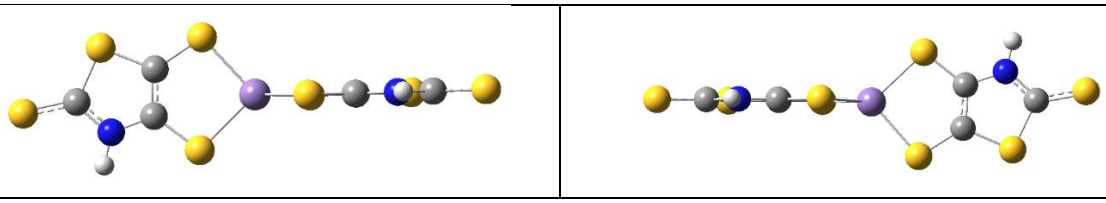

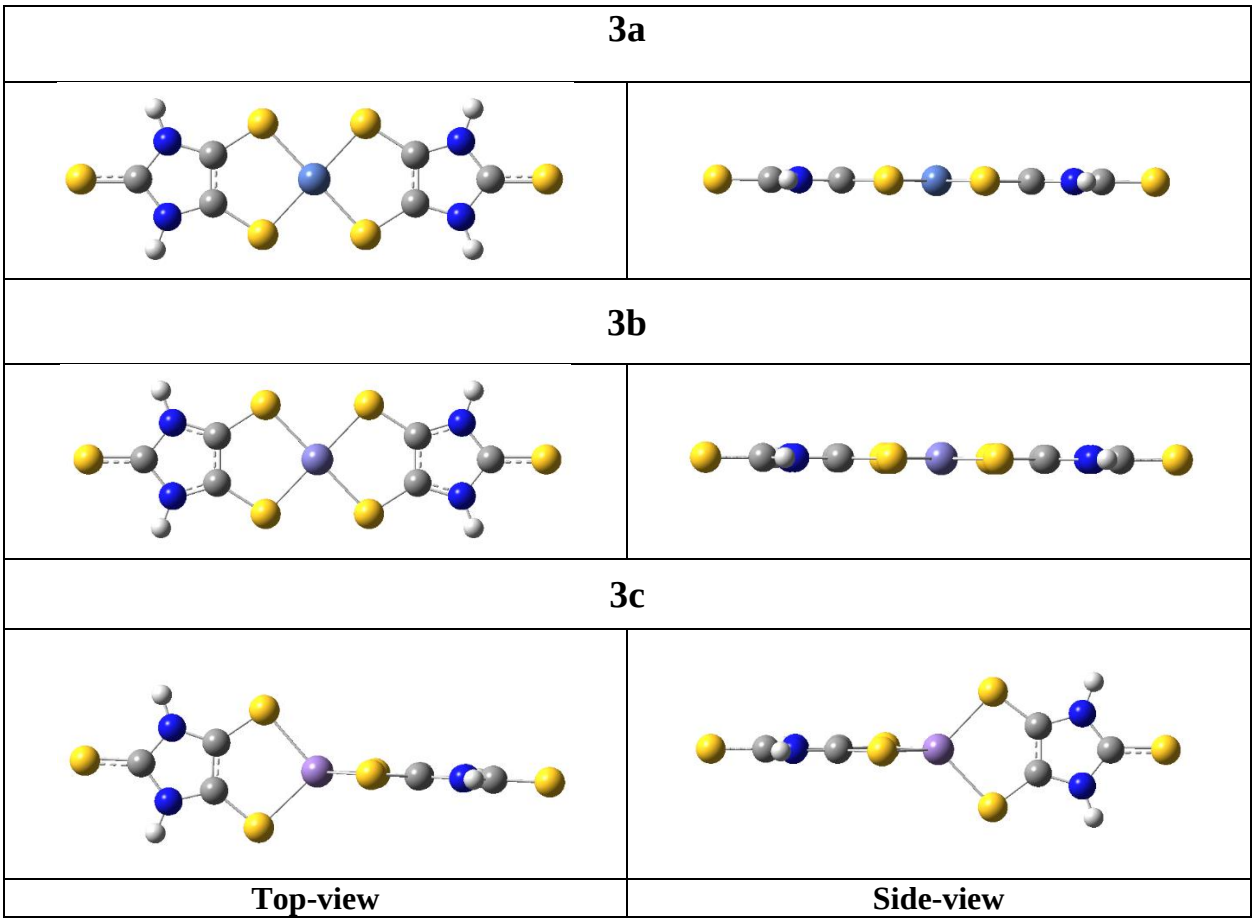

Figure S4 The shapes of all complexes **1a-3a**, **1b-3b** and **1c-3c** obtained at PBE/6-31G(d,p) level of theory