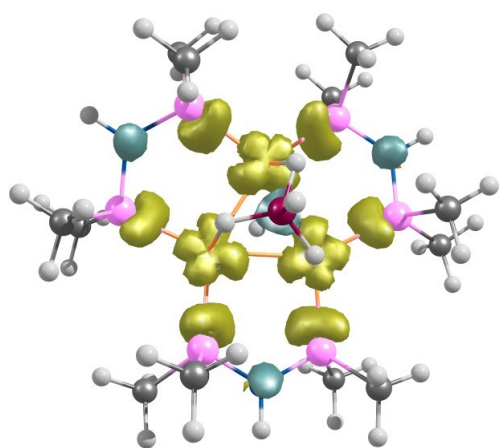


Supplementary information

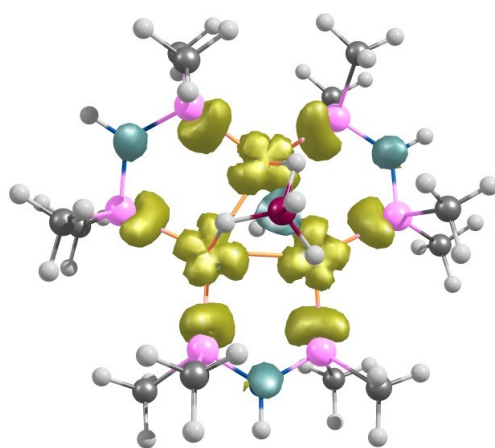
Electronic and Optical Properties of Copper Nanostructures for Advanced Applications

Ragheb Khalil Bouriche^{a,b}, Douniazed Hannachi^{c,d}, Amel Messai^a, Christophe Morell^e, Amor Azizi^b, Henry Chermette^{e*}

A

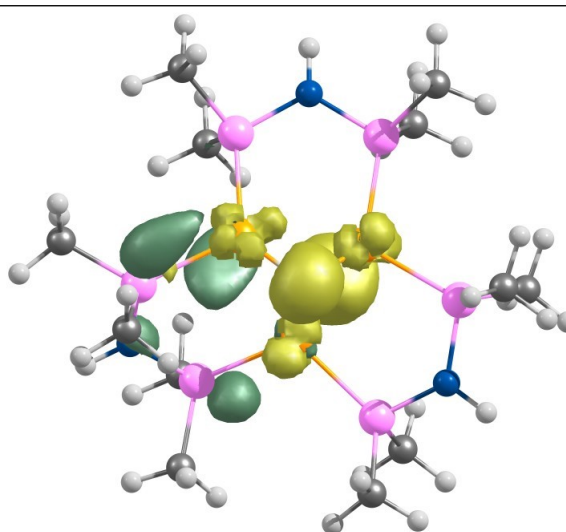


S1

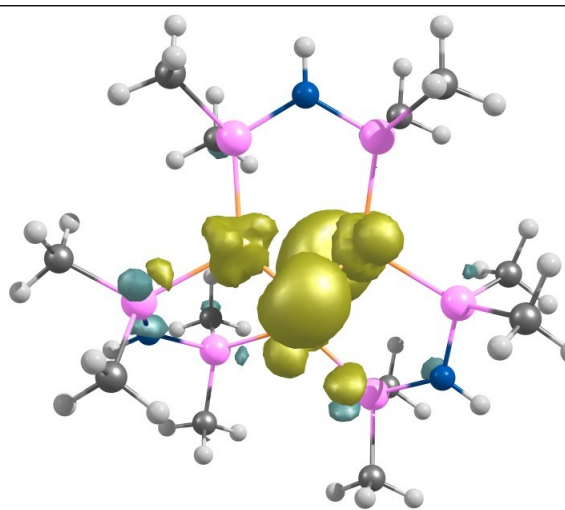


S10

B

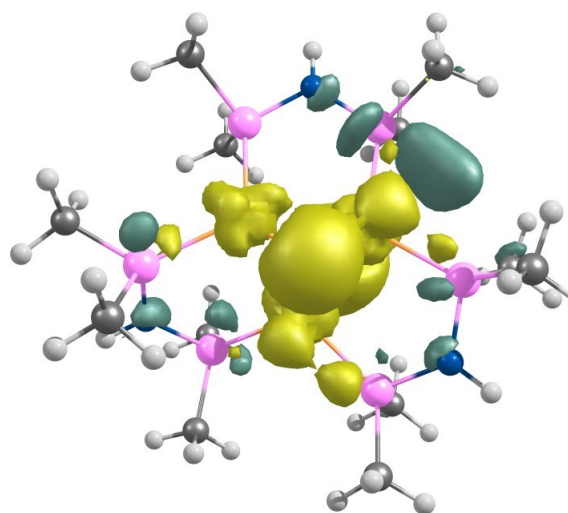


S1

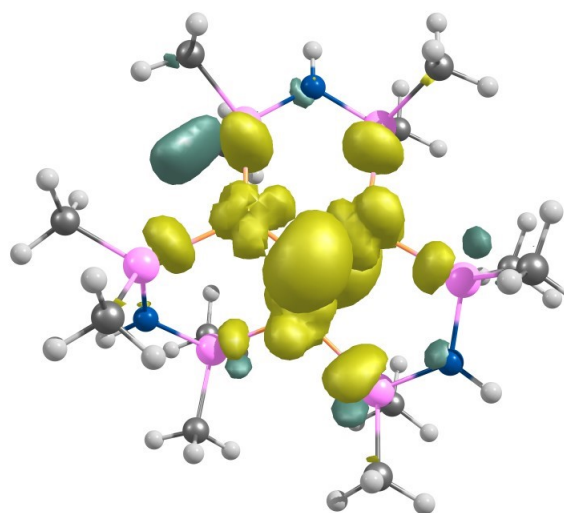


S5

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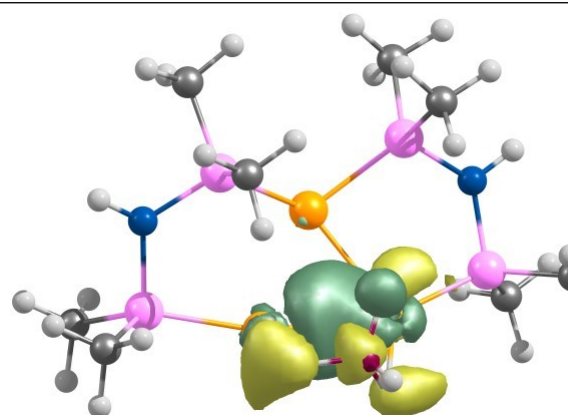


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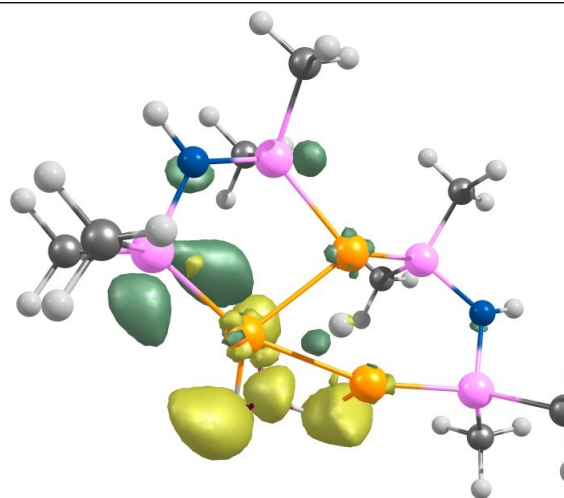


S19

C

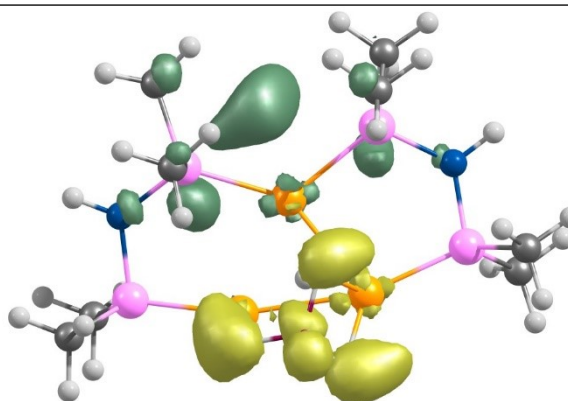


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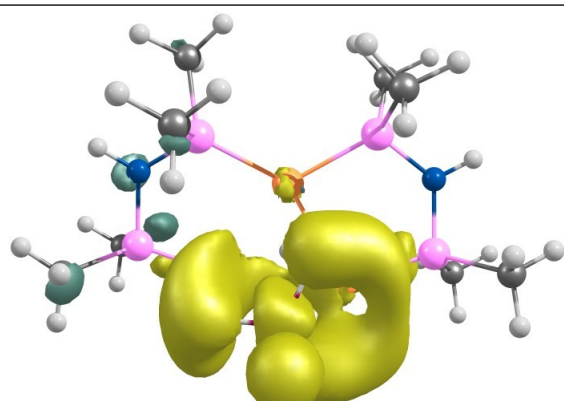


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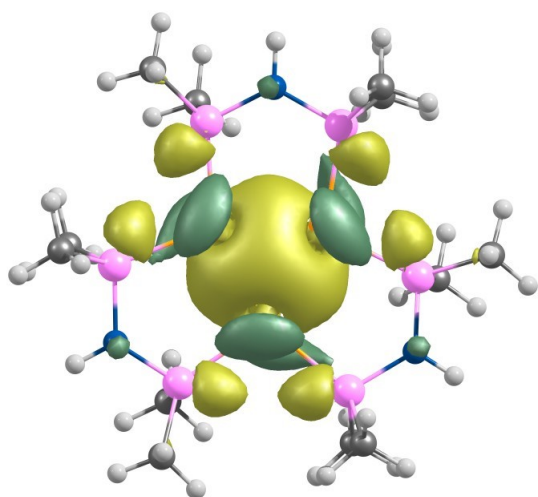


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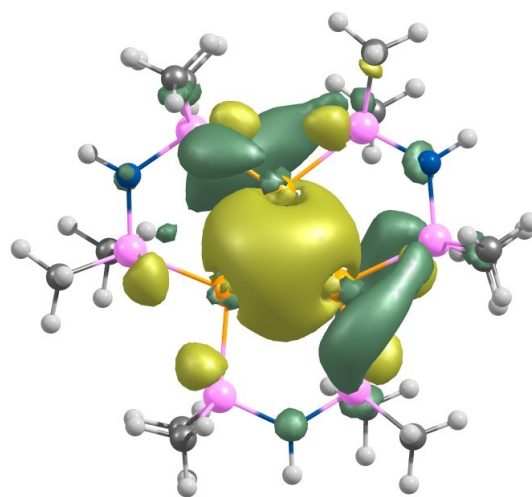


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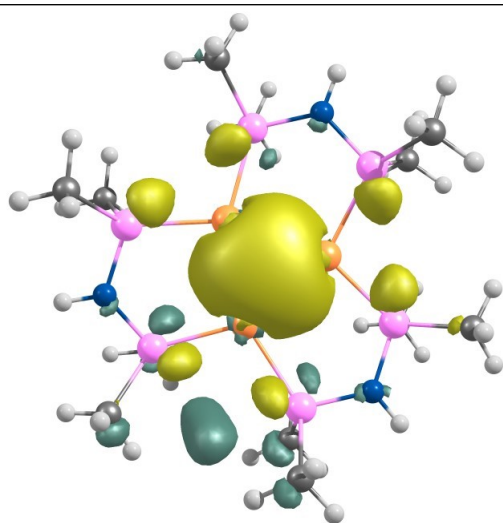
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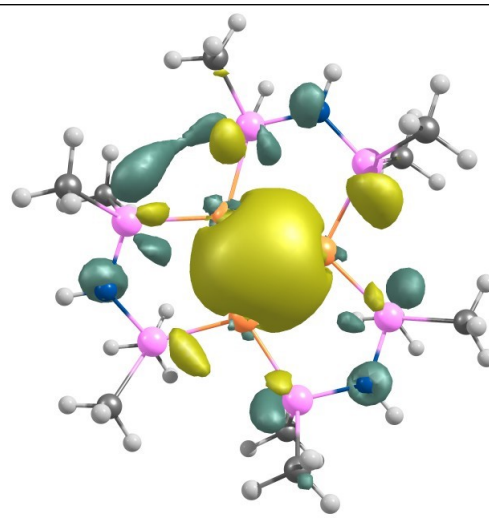
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S2

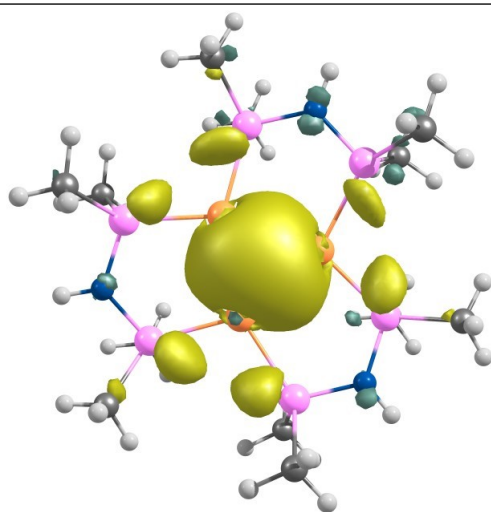


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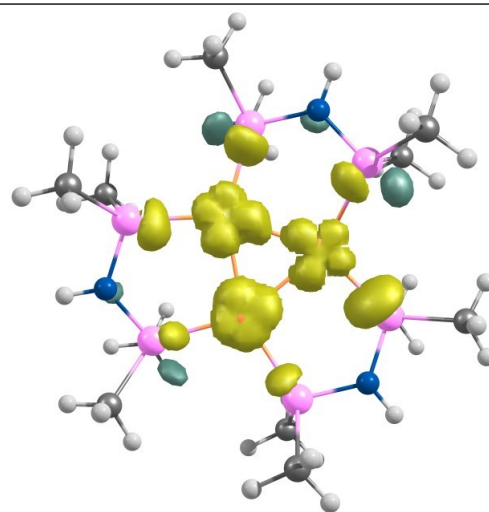


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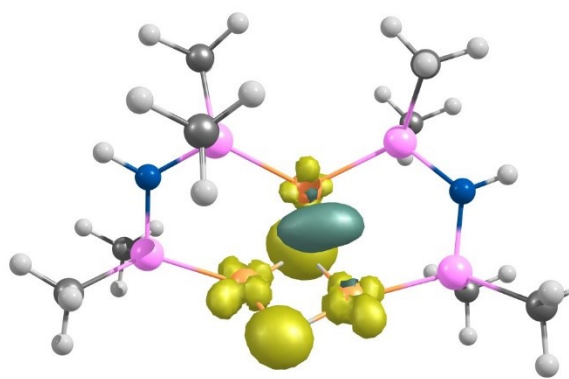


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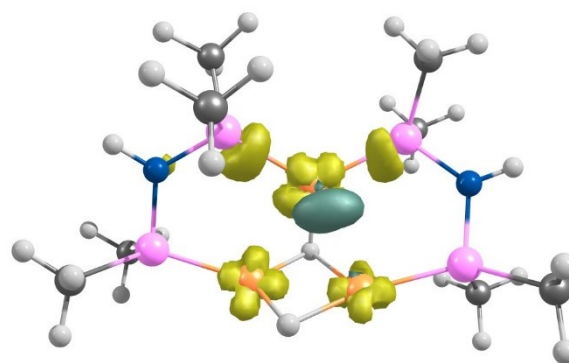


S15

E

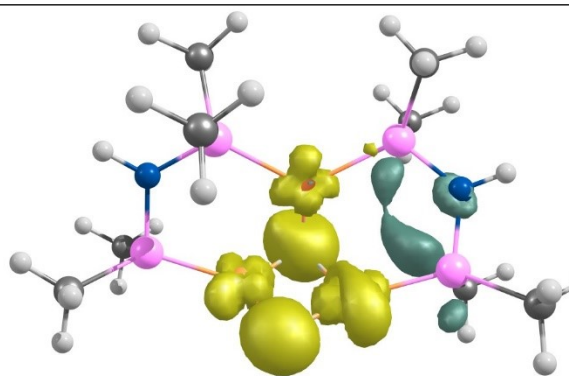


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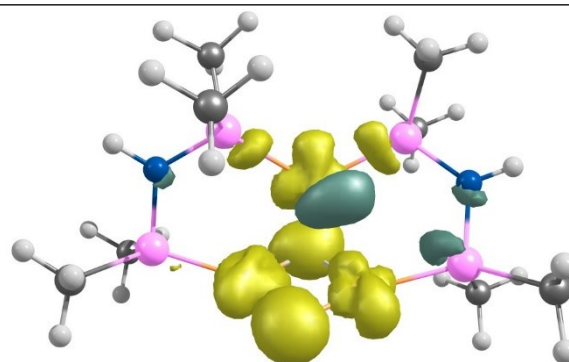


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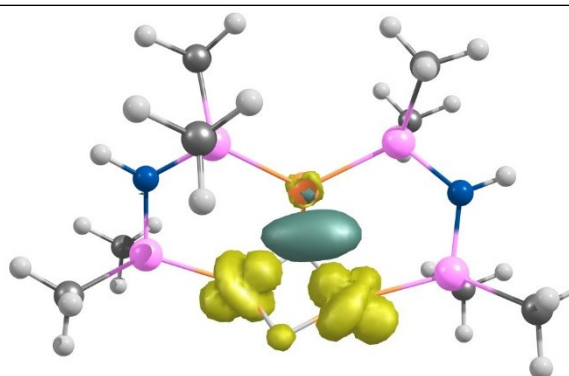


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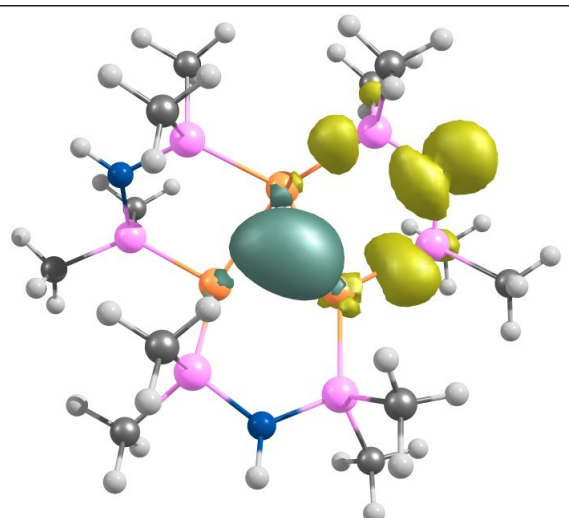
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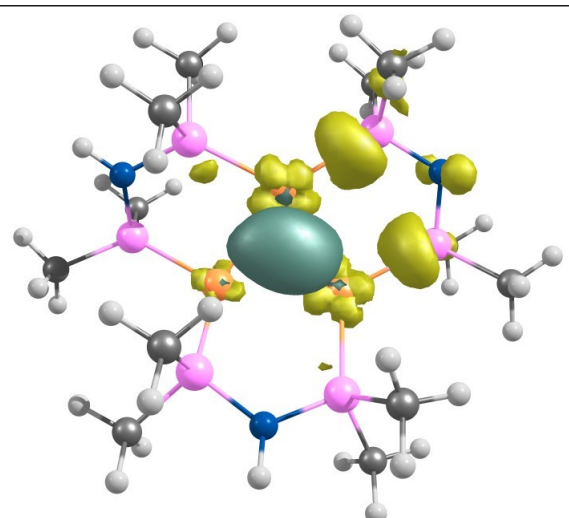


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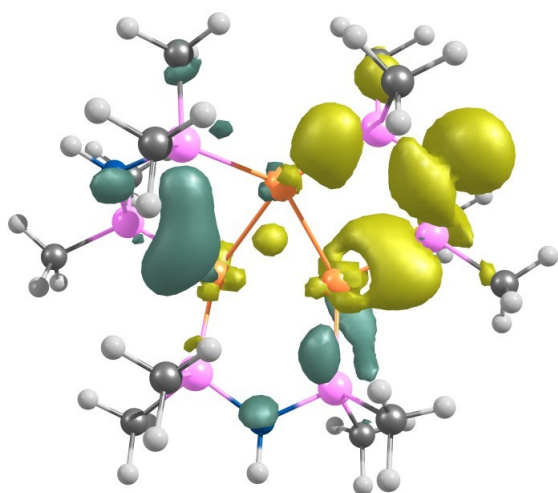
F



S1

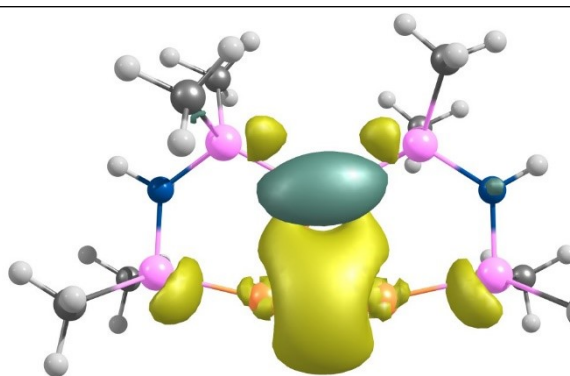


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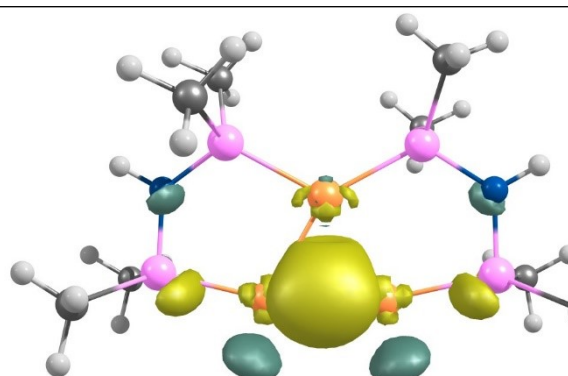


S6

G

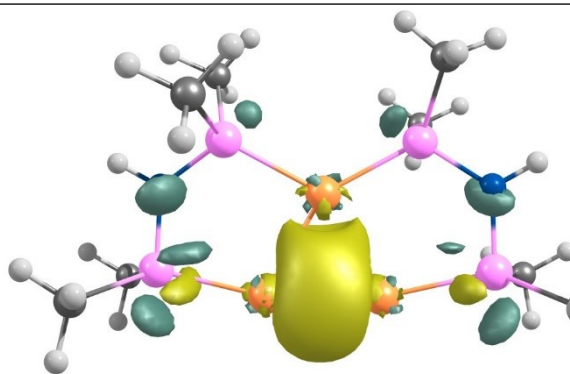


S1



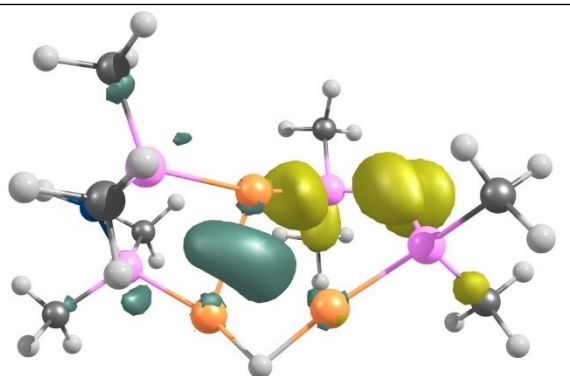
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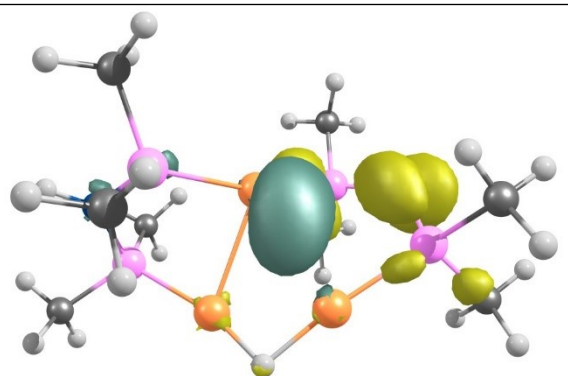


S4

H



S1



S2

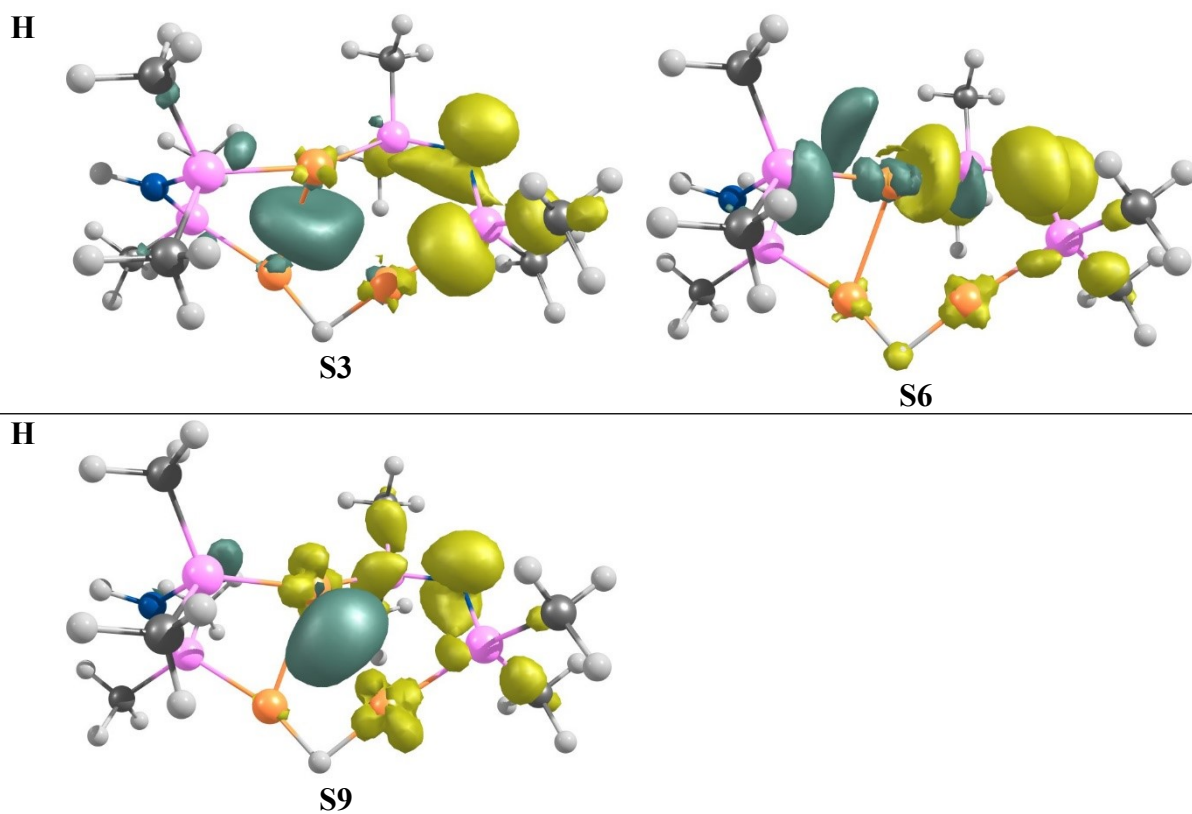
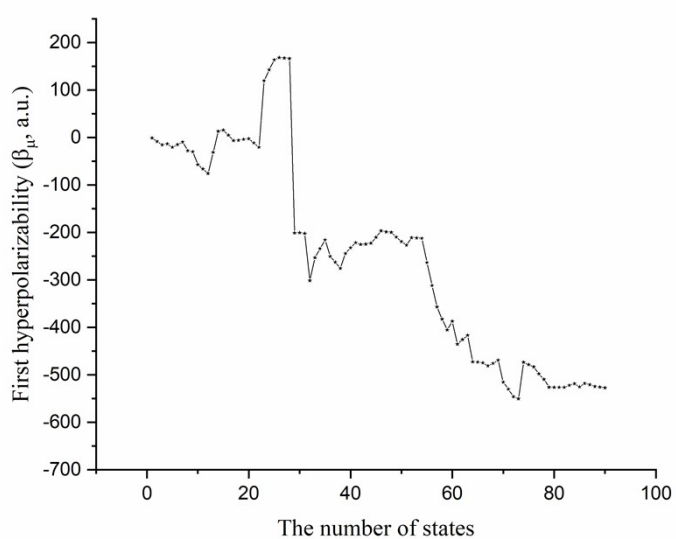
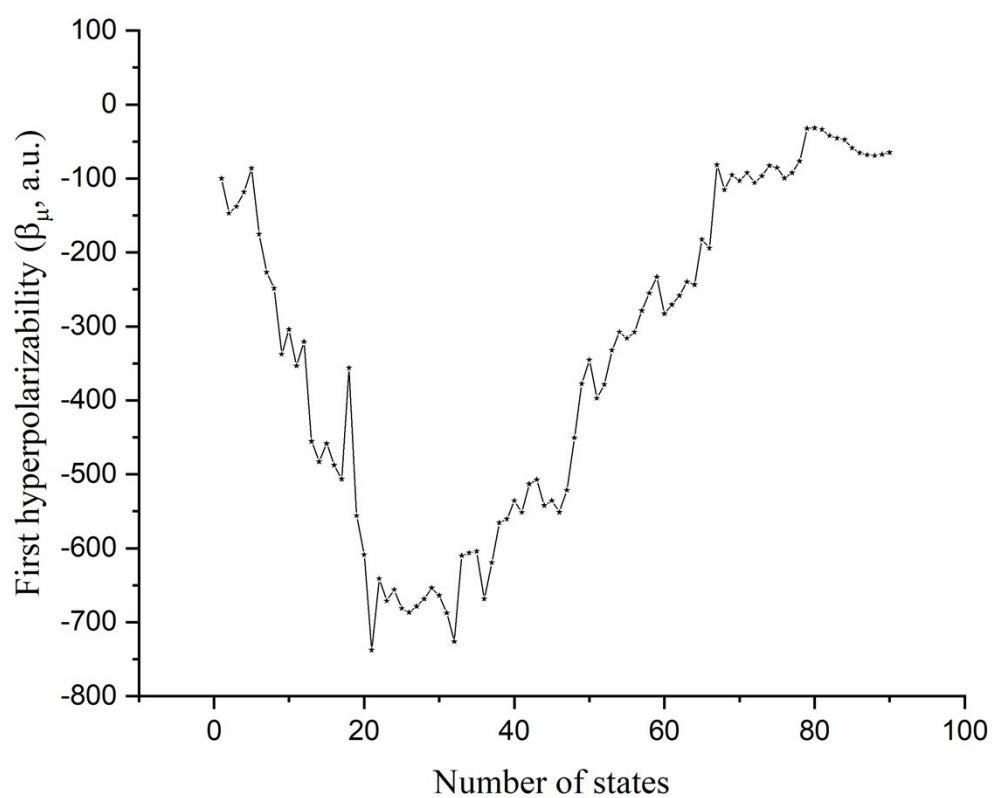


Figure S1 CDD for the crucial excited state of **A** to **H** nanoclusters. CDD was calculated as a difference between the corresponding excited state and the ground state of the considered system using the M06-2X/6-31+G(d)/SDD level of theory (yellow = negative density and green = positive density)

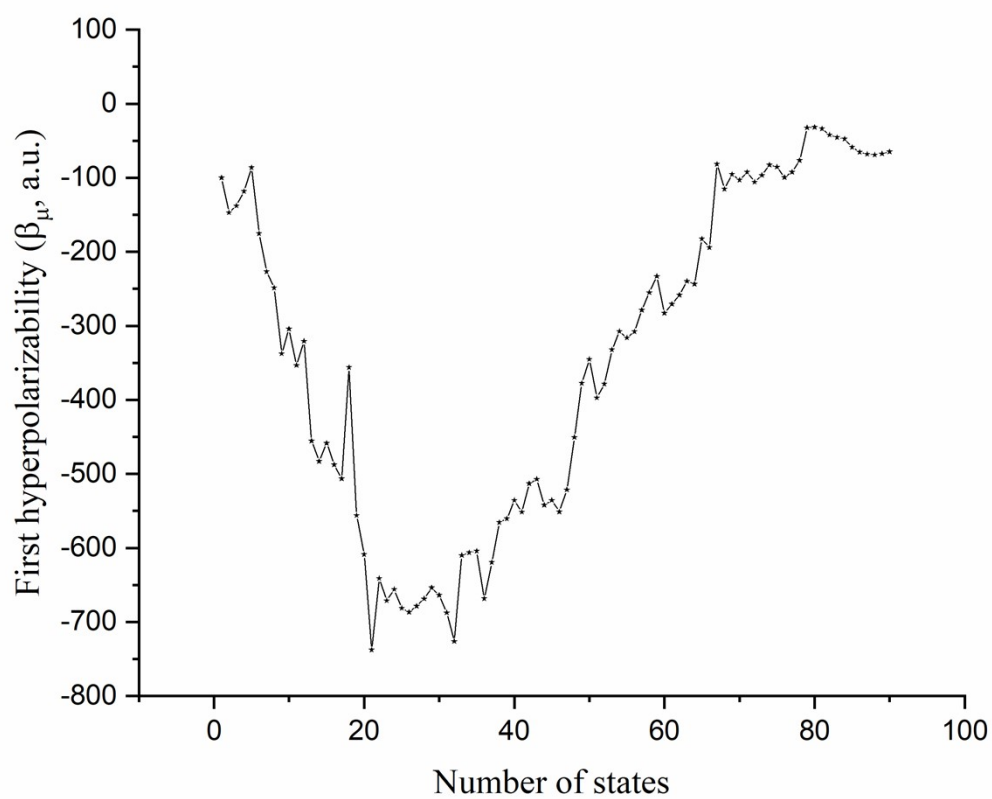
A



B



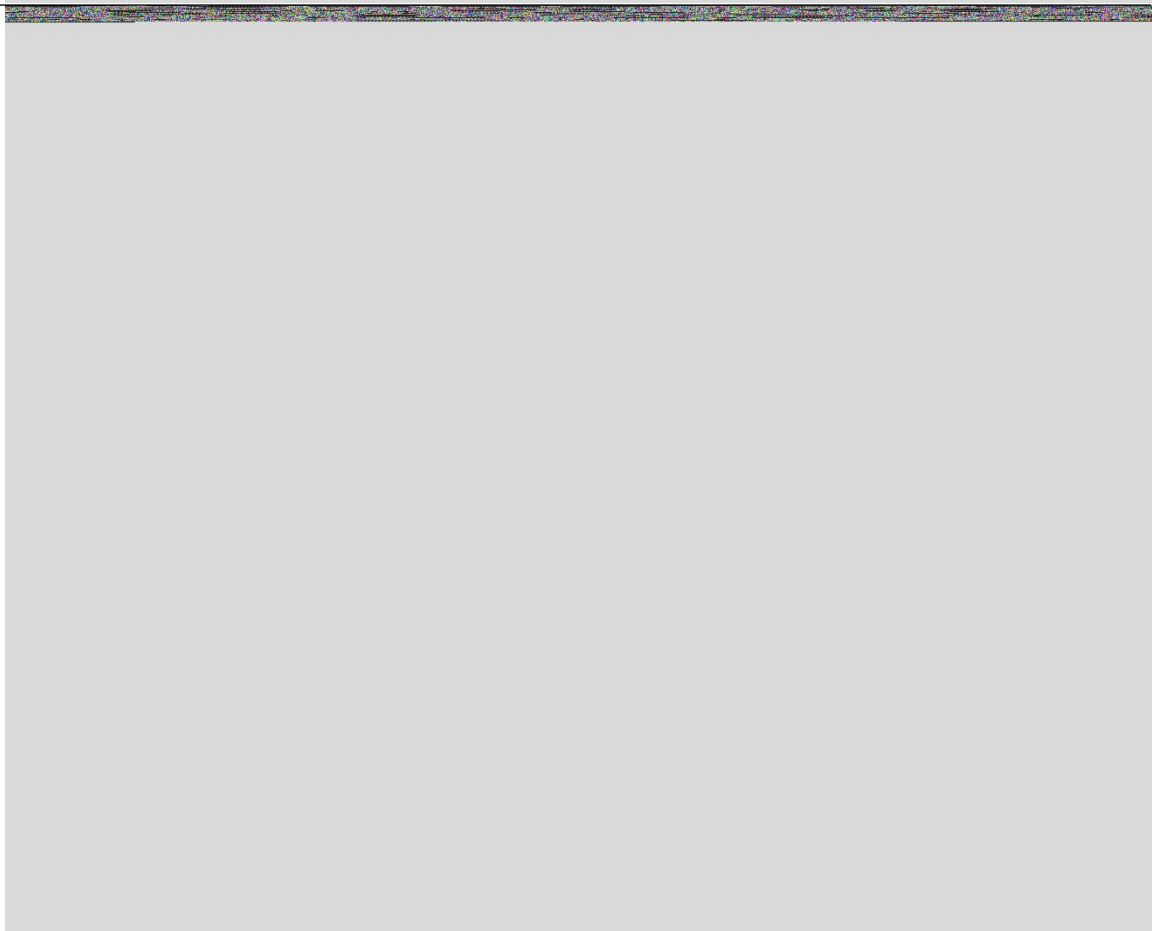
C



D



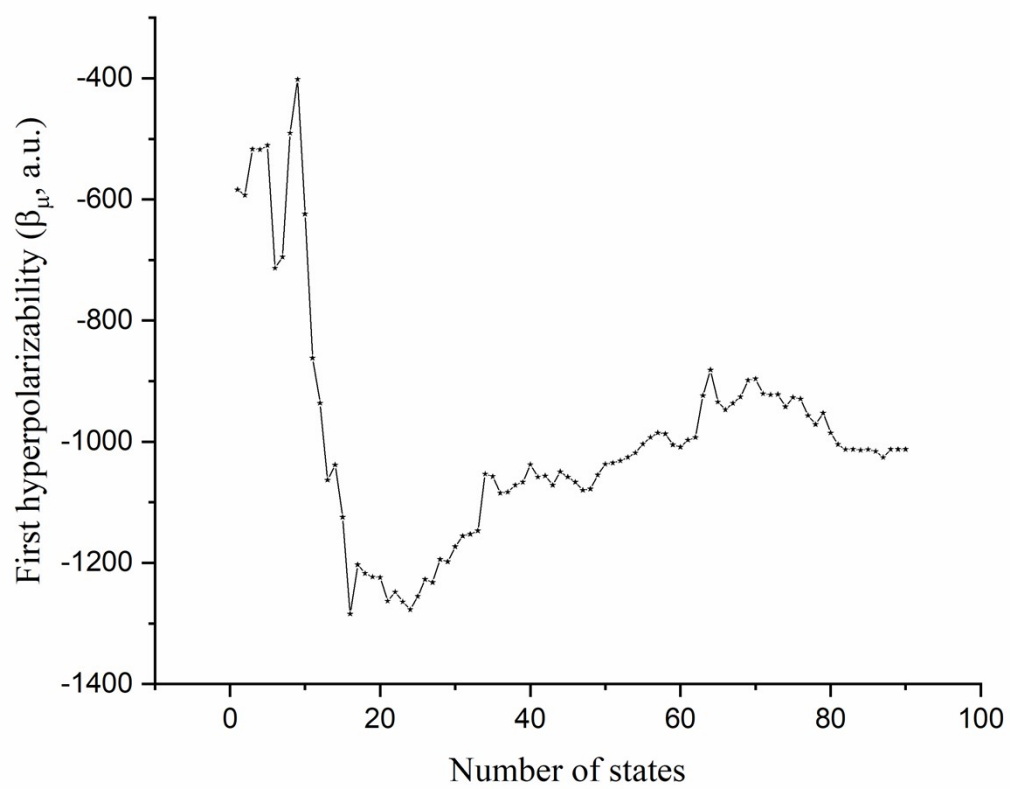
E



F



G



H

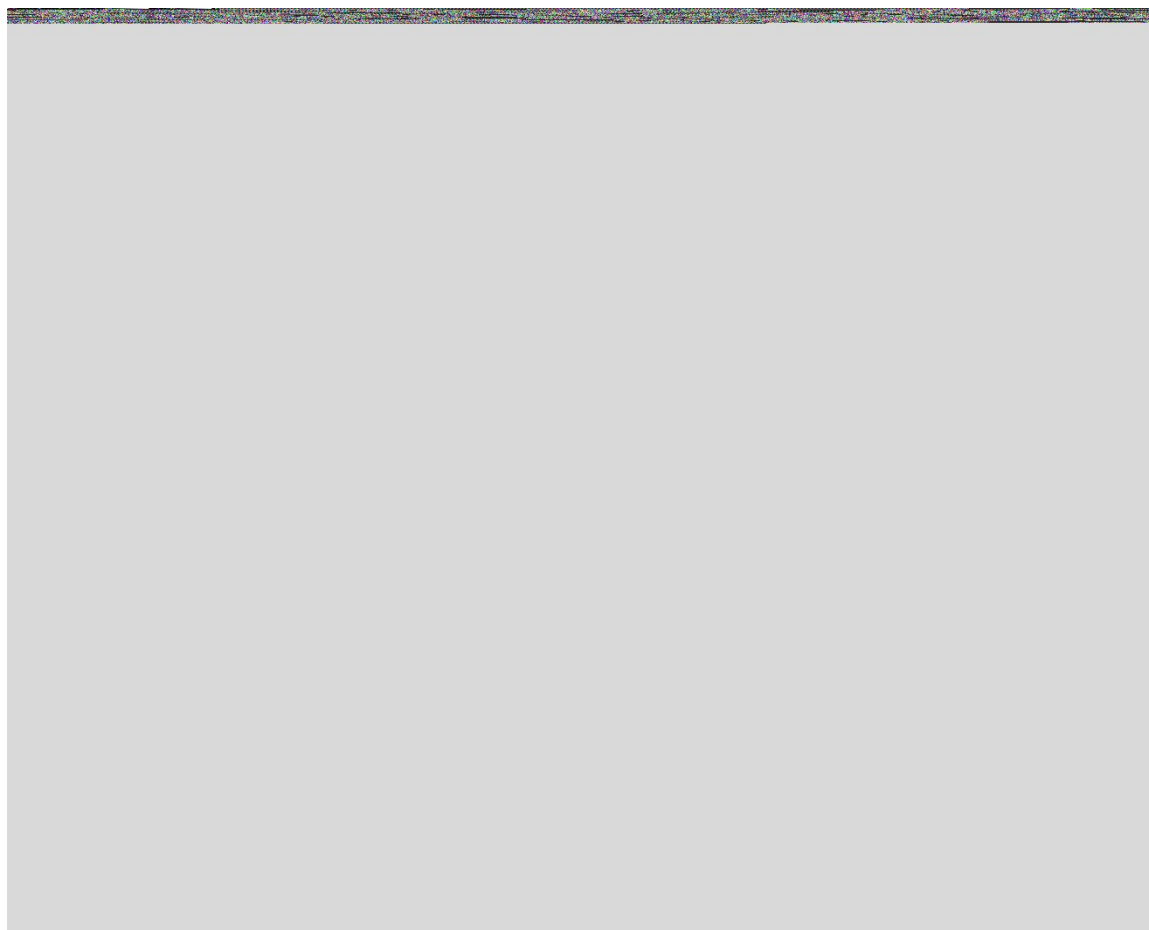


Figure S2 static first hyperpolarizability values calculated using the SOS formalism at the M06-2X/6-31+G(d)/SDD level of theory for **A** to **H** copper hydride nanoclusters