

Supporting Information for Geometric structure, electronic and spectral properties of metal-free phthalocyanine under the external electric fields

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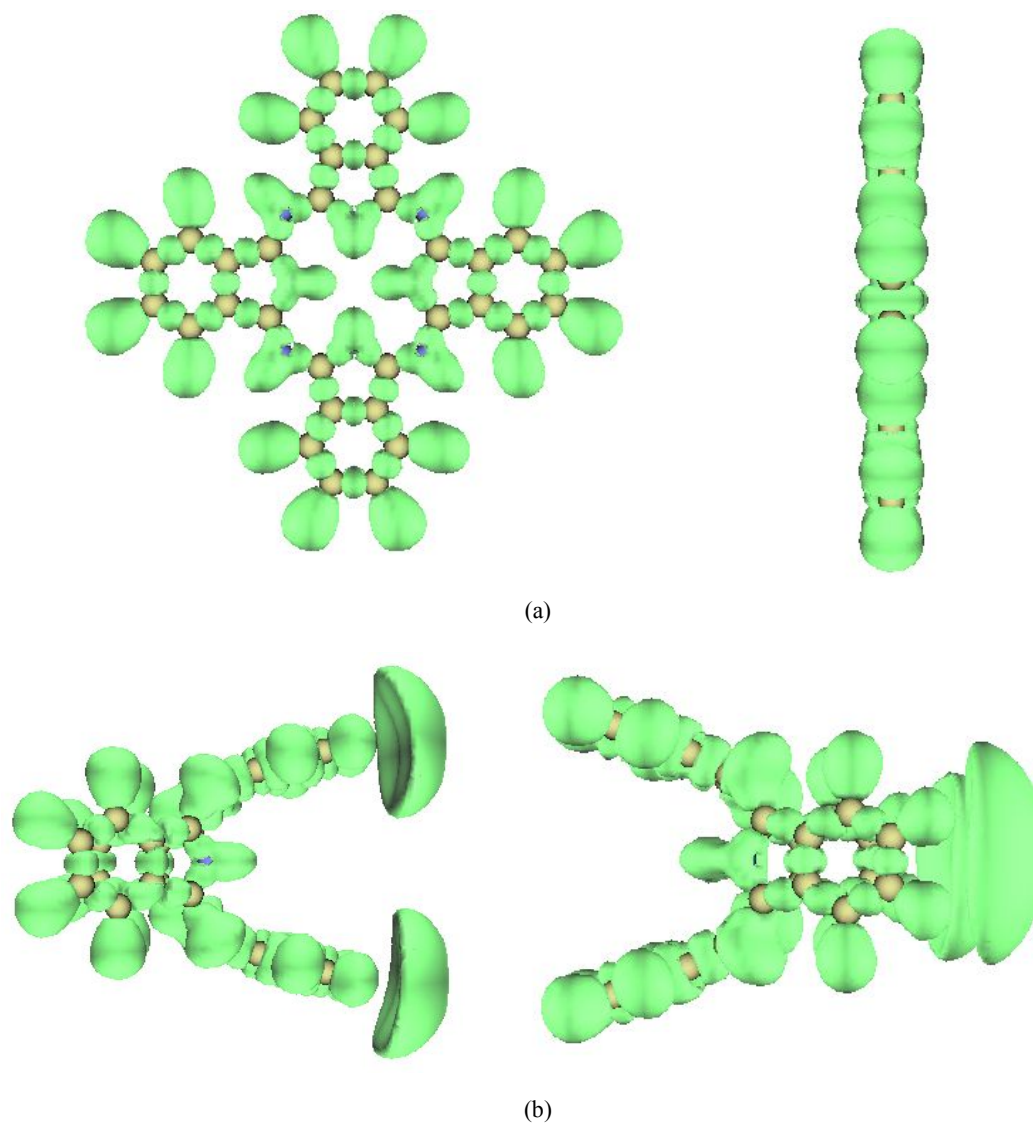


Figure S1. Electron localization function (ELF) with the isovalue set to 0.70. (a) EEF is 0 a.u., the left is observed along the x direction and the right is observed along the z direction, and (b) EEF is -0.025 a.u., the left is observed along the y direction and the right is observed along the z direction.

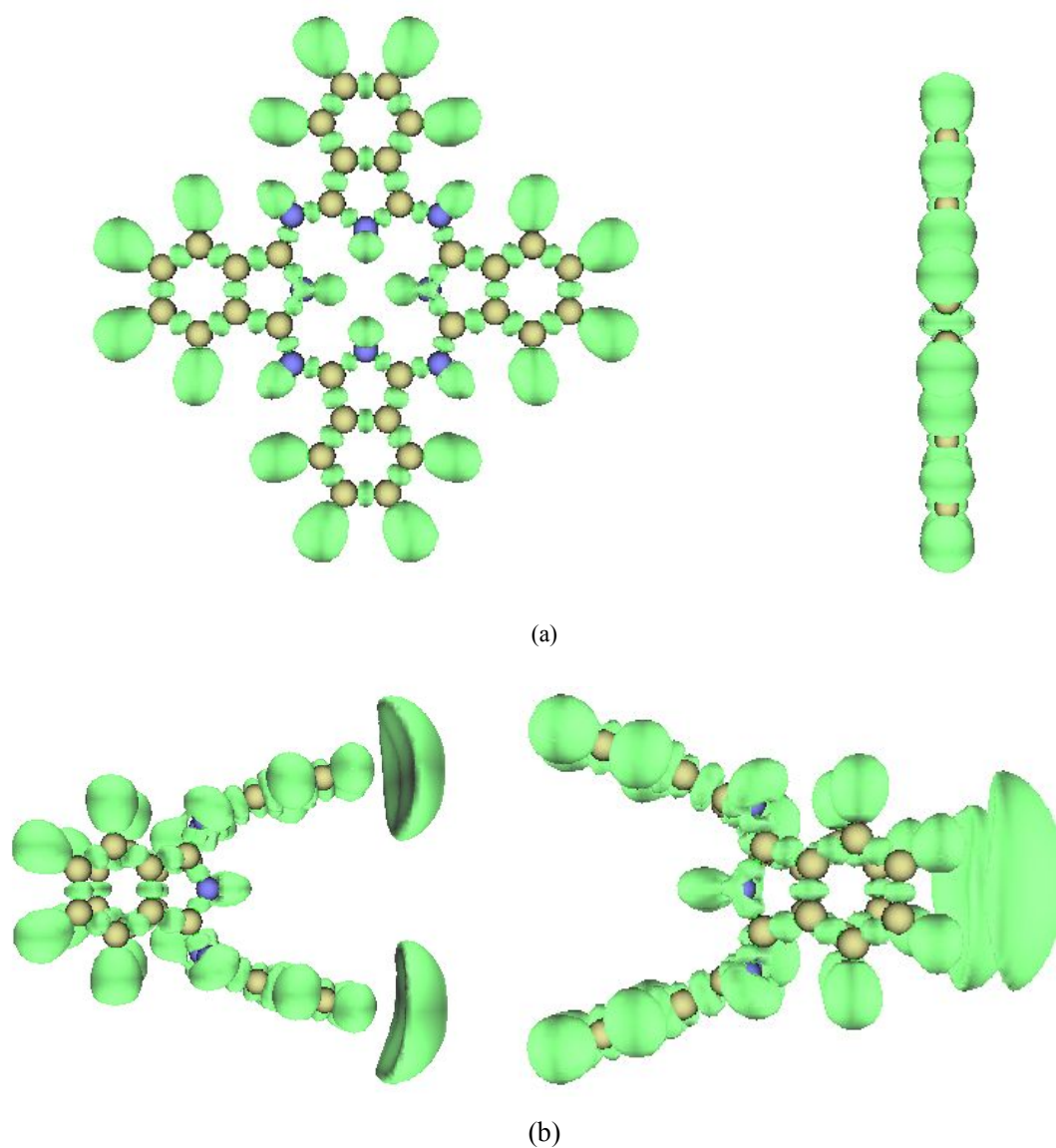
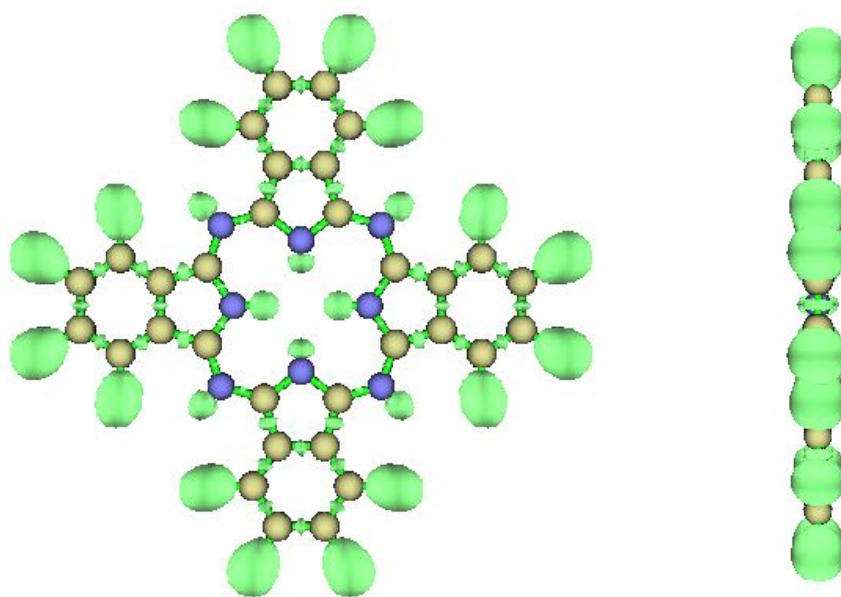
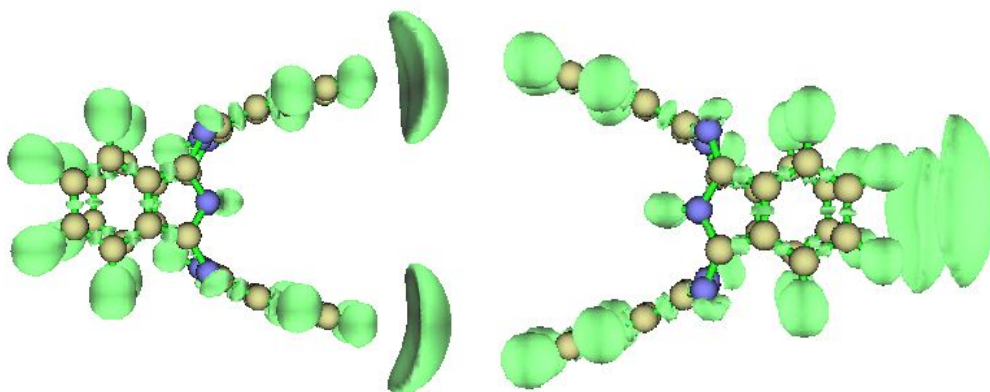


Figure S2. Electron localization function (ELF) with the isovalue set to 0.80. (a) EEF is 0 a.u., the left is observed along the x direction and the right is observed along the z direction, and (b) EEF is -0.025 a.u., the left is observed along the y direction and the right is observed along the z direction.

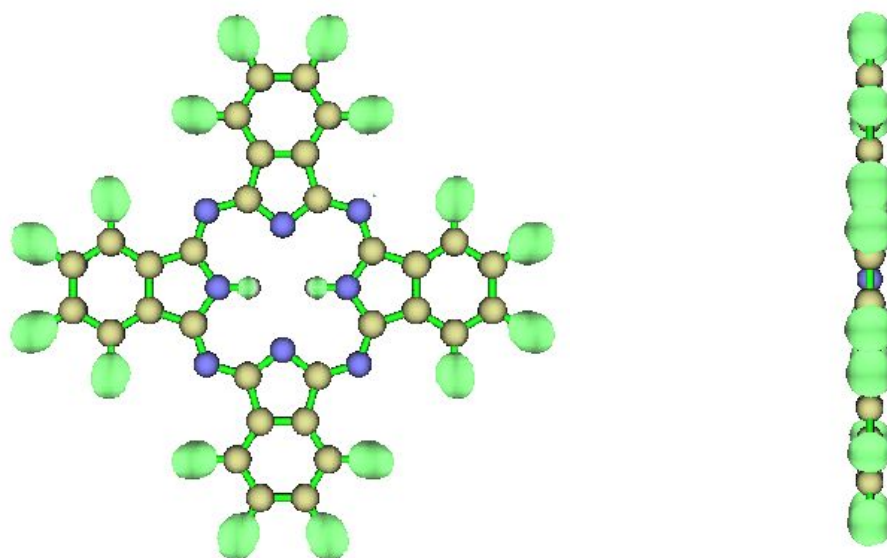


(a)

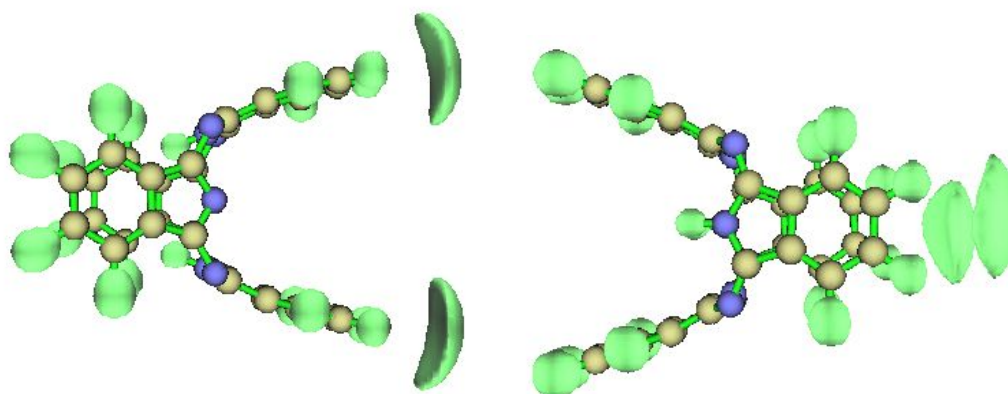


(b)

Figure S3. Electron localization function (ELF) with the isovalue set to 0.90. (a) EEF is 0 a.u., the left is observed along the x direction and the right is observed along the z direction, and (b) EEF is -0.025 a.u., the left is observed along the y direction and the right is observed along the z direction.



(a)



(b)

Figure S4. Electron localization function (ELF) with the isovalue set to 0.96. (a) EEF is 0 a.u., the left is observed along the x direction and the right is observed along the z direction, and (b) EEF is -0.025 a.u., the left is observed along the y direction and the right is observed along the z direction.