Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Catalytic activity of corrole complexes with post-transition elements for oxidation of carbon monoxide: A first-principles study

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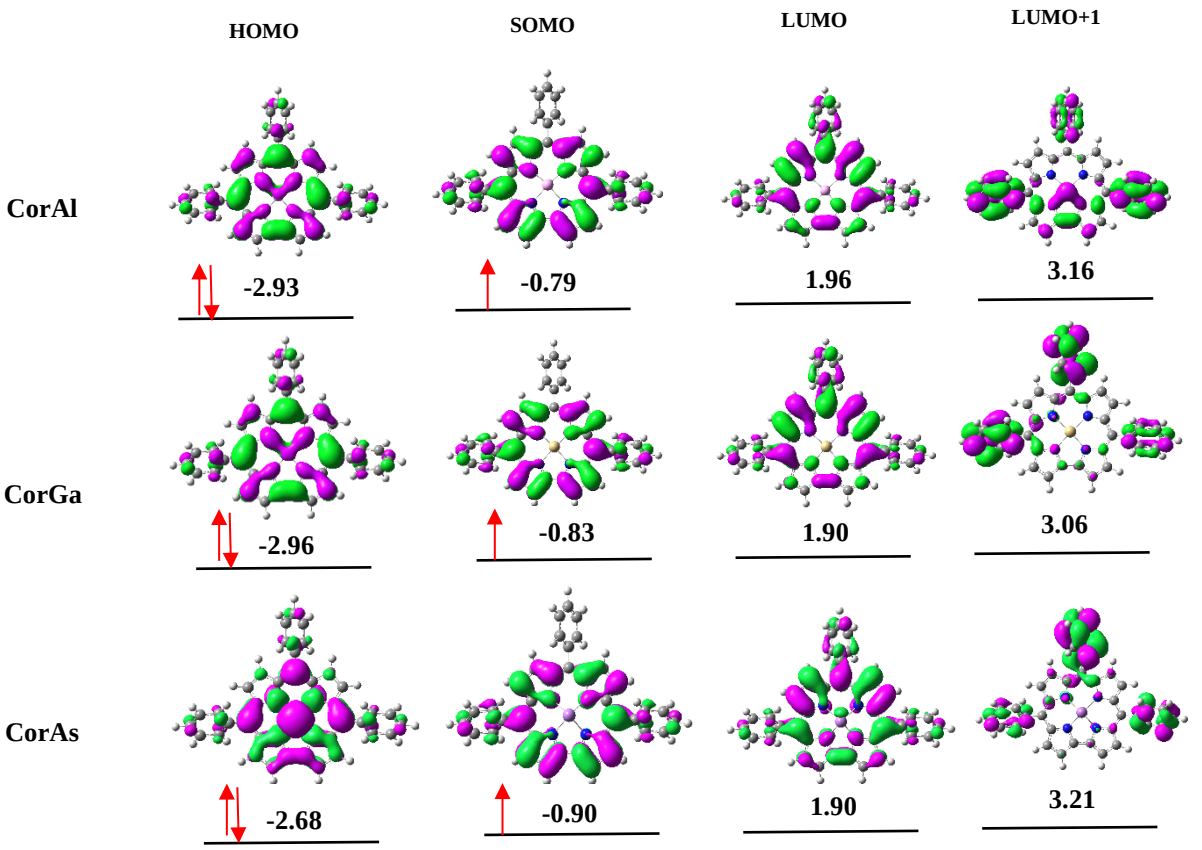
Frontier molecule orbitals for studied corrole complexes



Crystallographic Information File (CIF) for iodinated aluminum (III) corrole, which has similar structure to the corrole complexes that we have studied in our work, is available in supporting information of following article:

J. Vestfrid, M. Botoshansky, J. H. Palmer, A. C. Durrell, H. B. Gray and Z. Gross, *J. Am. Chem. Soc.*, 2011, **133**, 12899–12901.

(https://pubs.acs.org/doi/suppl/10.1021/ja202692b)

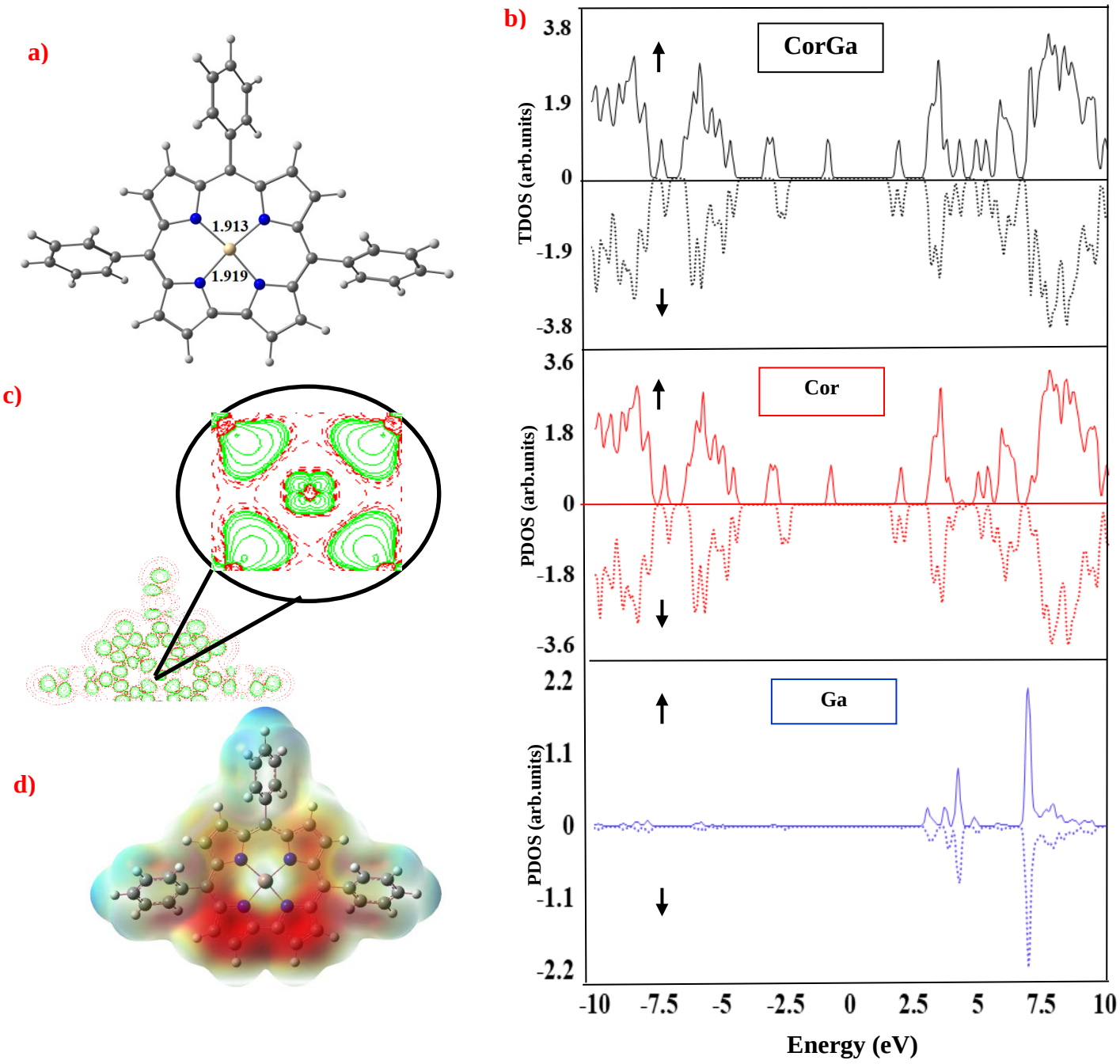


Fig. S1 Calculated properties for of CorGa. a) The optimized structure with the bond distances in Å, b) Spin-polarized TDOS and PDOS, c) The contour plot of electron deformation density, d) The molecular electrostatic potential isosurface (0.0004 au).

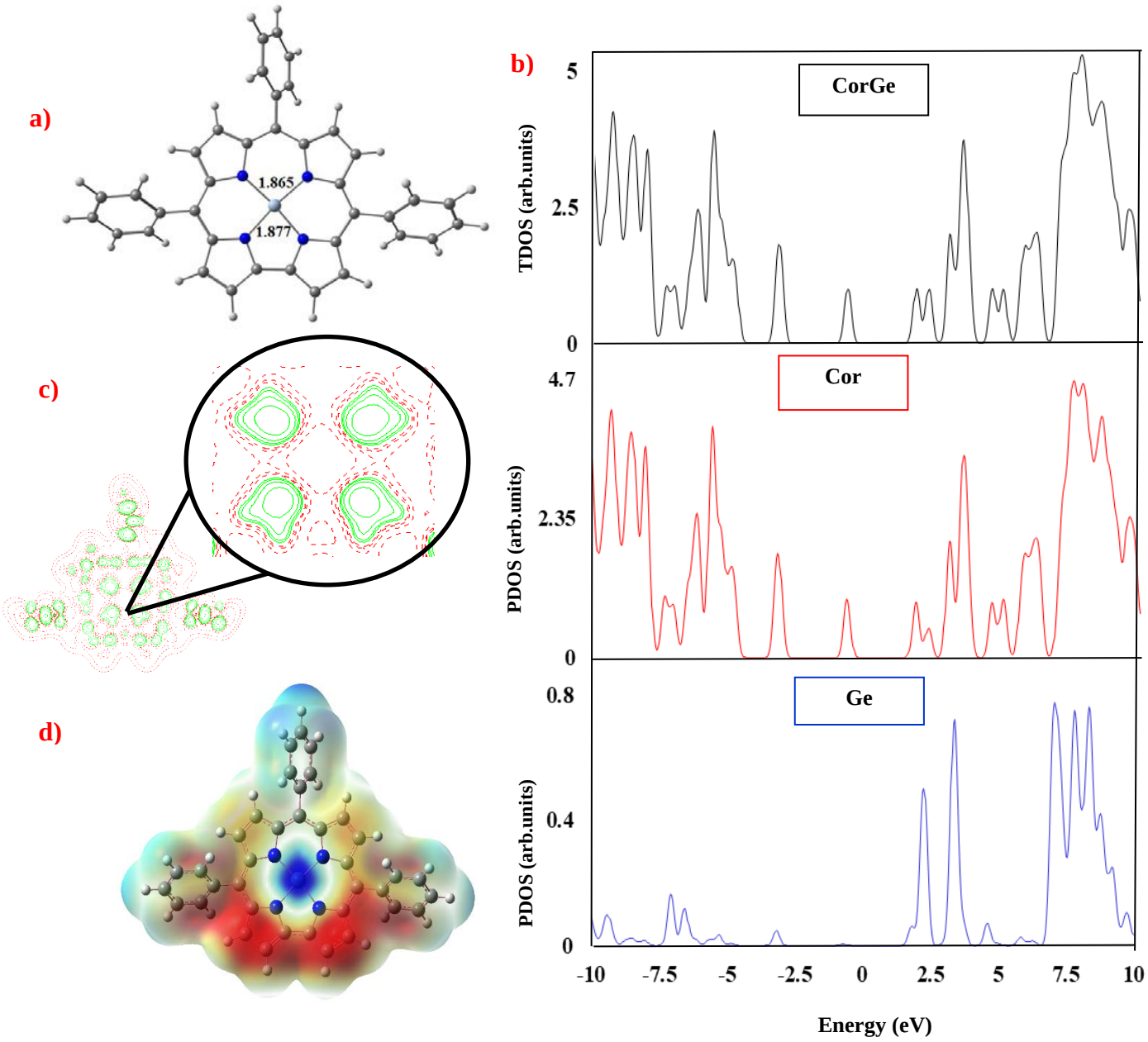


Fig. S2 Calculated properties for of CorGe. a) The optimized structure with the bond distances in Å, b) TDOS and PDOS, c) The contour plot of electron deformation density, d) The molecular electrostatic potential isosurface (0.0004 au

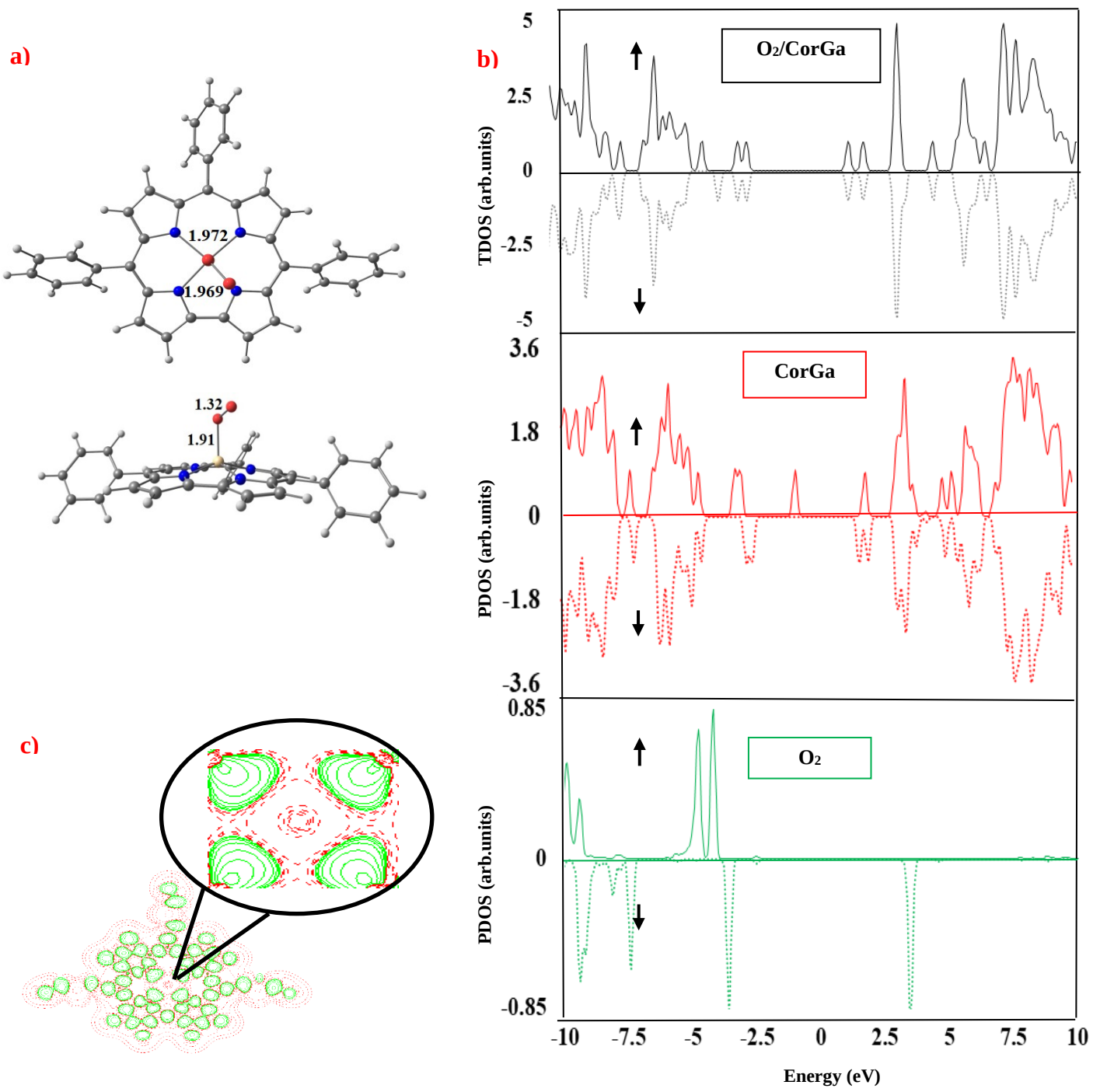


Fig. S3. Calculated properties for the most stable configuration of O_2 adsorption on CorGa. a) Top and side views of the optimized structure with the bond distances in Å, b) Spin-polarized TDOS and PDOS, c) The contour plot of electron deformation density.

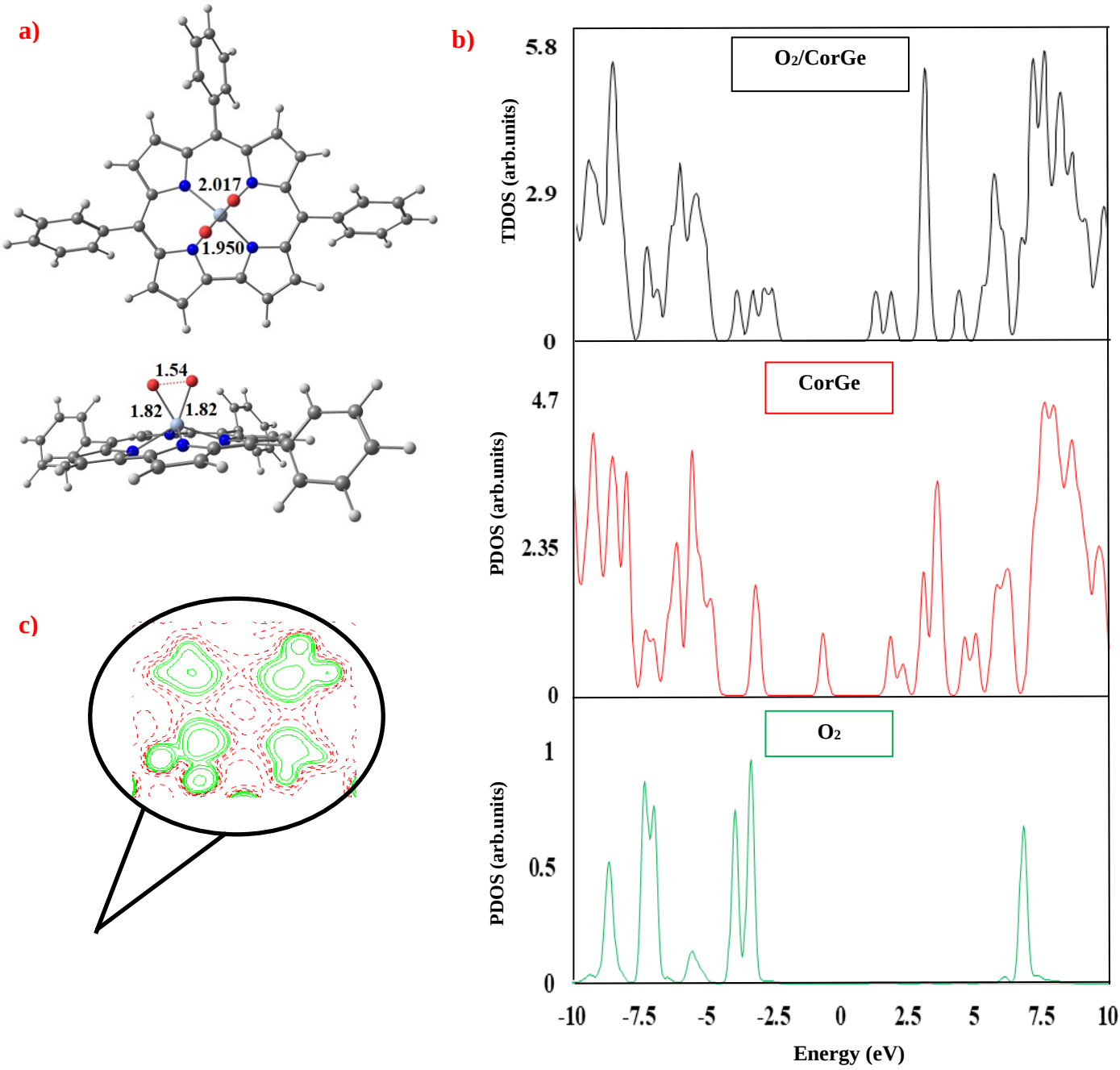


Fig. S4 Calculated properties for the most stable configuration of O_2 adsorption on CorGe. a) Top and side views of the optimized structure with the bond distances in Å, b) Spin-polarized TDOS and PDOS, c) The contour plot of electron deformation density.

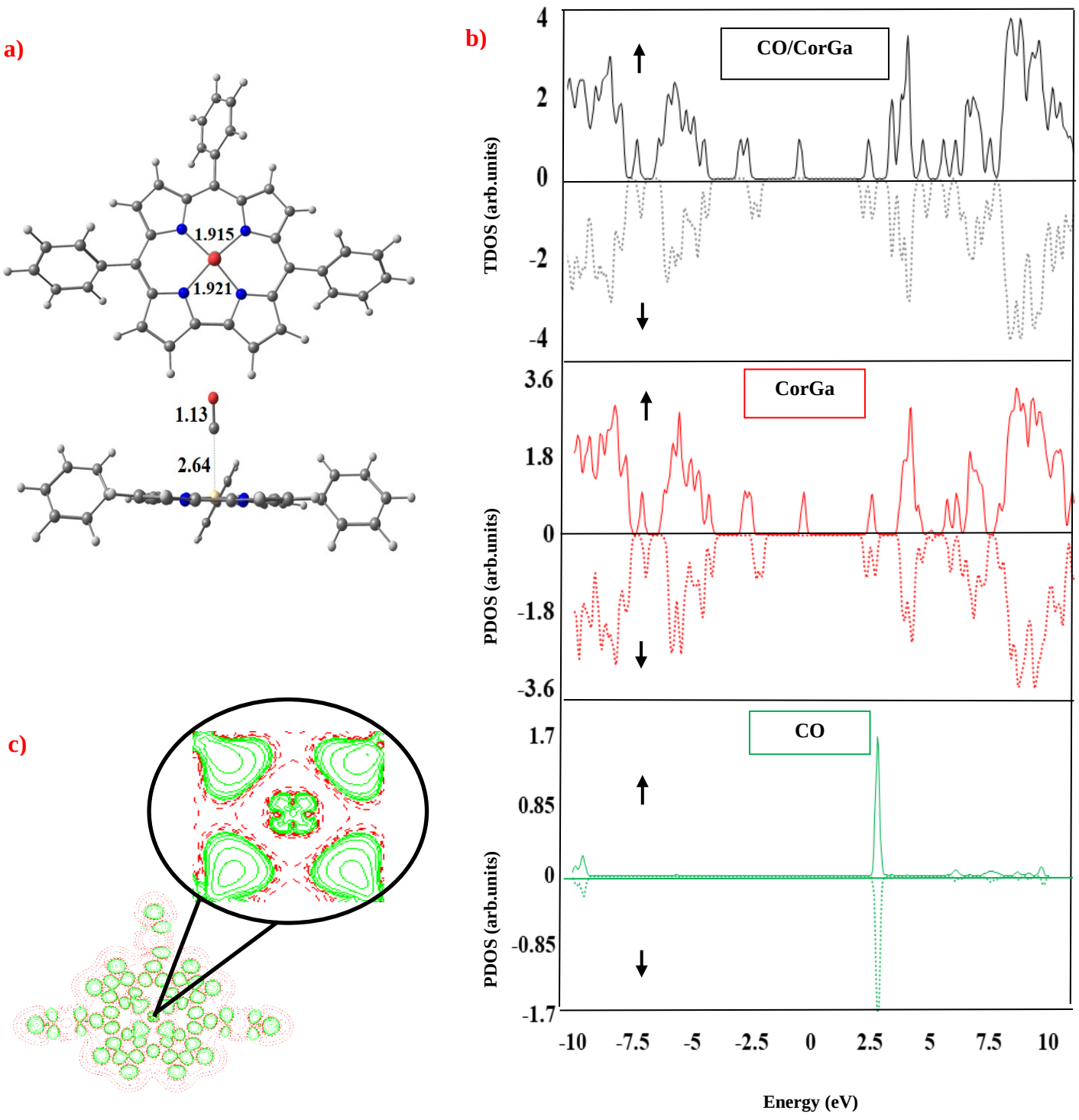


Fig S5 Calculated properties for the most stable configuration of CO adsorption on CorGa. a) Top and side views of the optimized structure with the bond distances in Å, b) Spin-polarized TDOS and PDOS, c) The contour plot of electron deformation density.

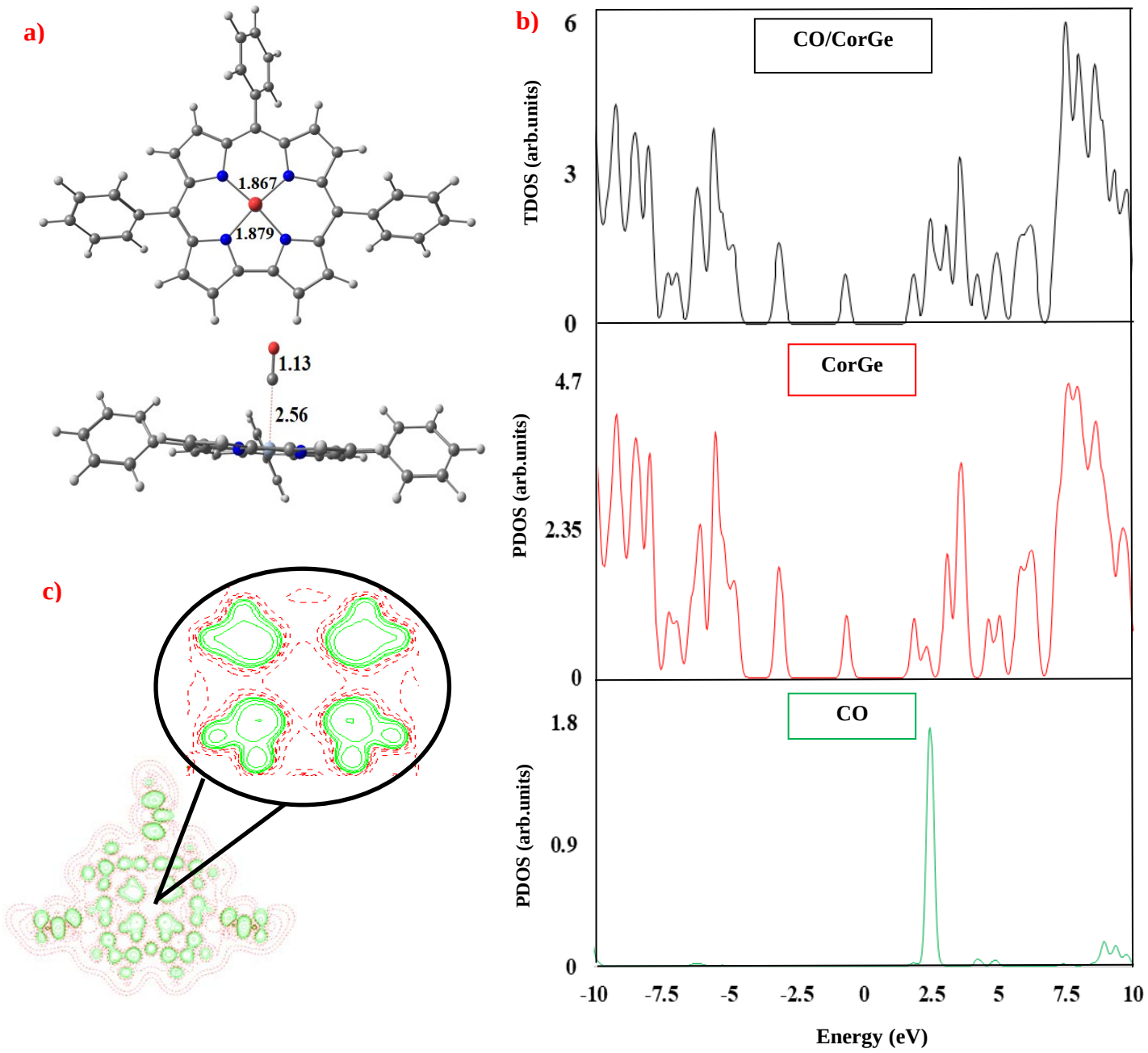


Fig S6. Calculated properties for the most stable configuration of CO adsorption on CorGe. a) Top and side views of the optimized structure with the bond distances in Å, b) Spin-polarized TDOS and PDOS, c) The contour plot of electron deformation density.

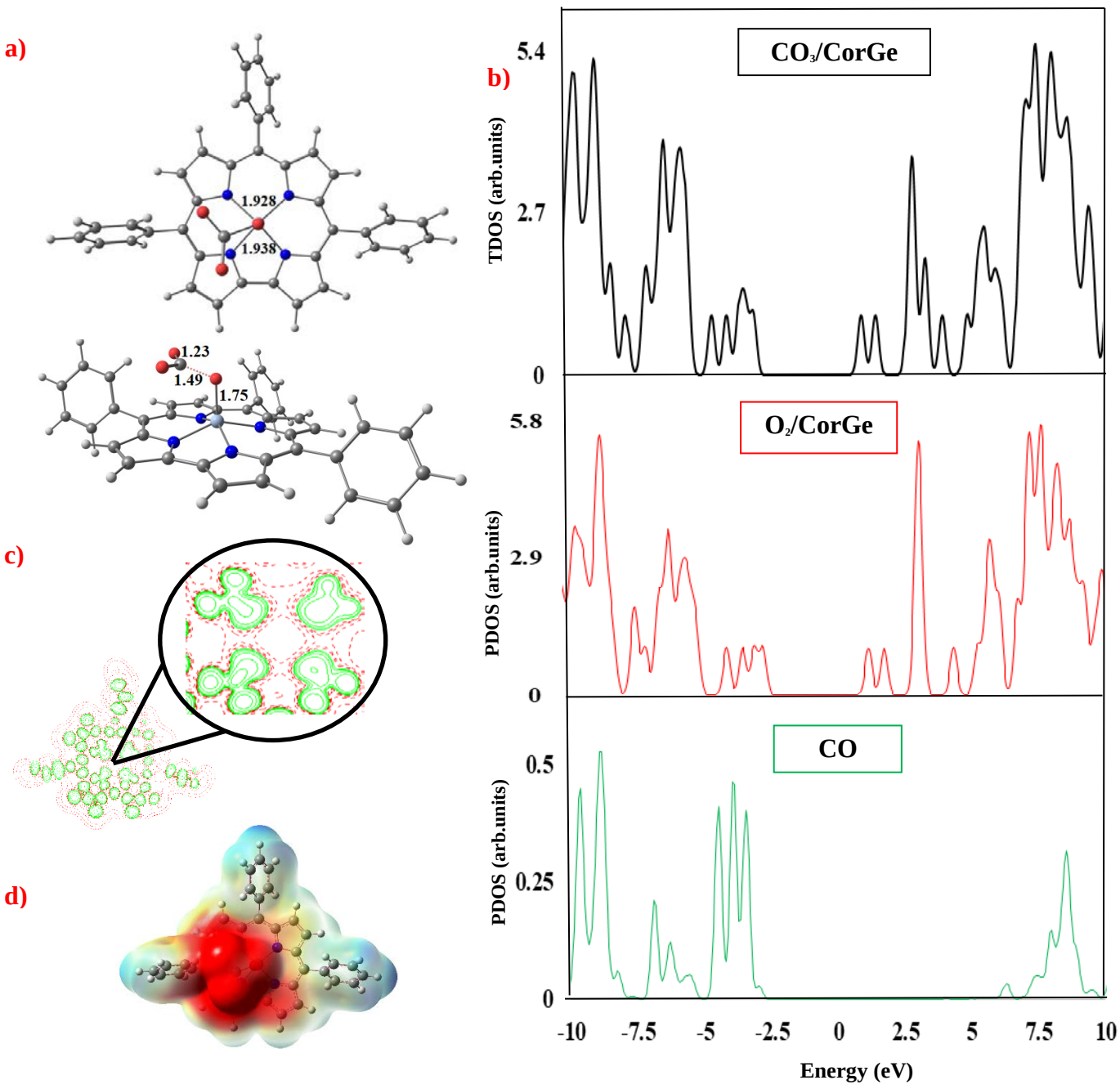


Fig S7. Calculated properties for the most stable configuration of co-adsorption of O_2 and CO on CorGe. a) The top and side views of optimized structure with the bond distances in Å, b) TDOS and PDOS, c) The contour plot of electron deformation density, d) The molecular electrostatic potential isosurface (0.0004 au).