

Supporting Information for

Study of the Molecular Properties of Mono and Binuclear Metal *s*-Indacenyl Complexes with Ir, Rh and Re: A Theoretical Approach

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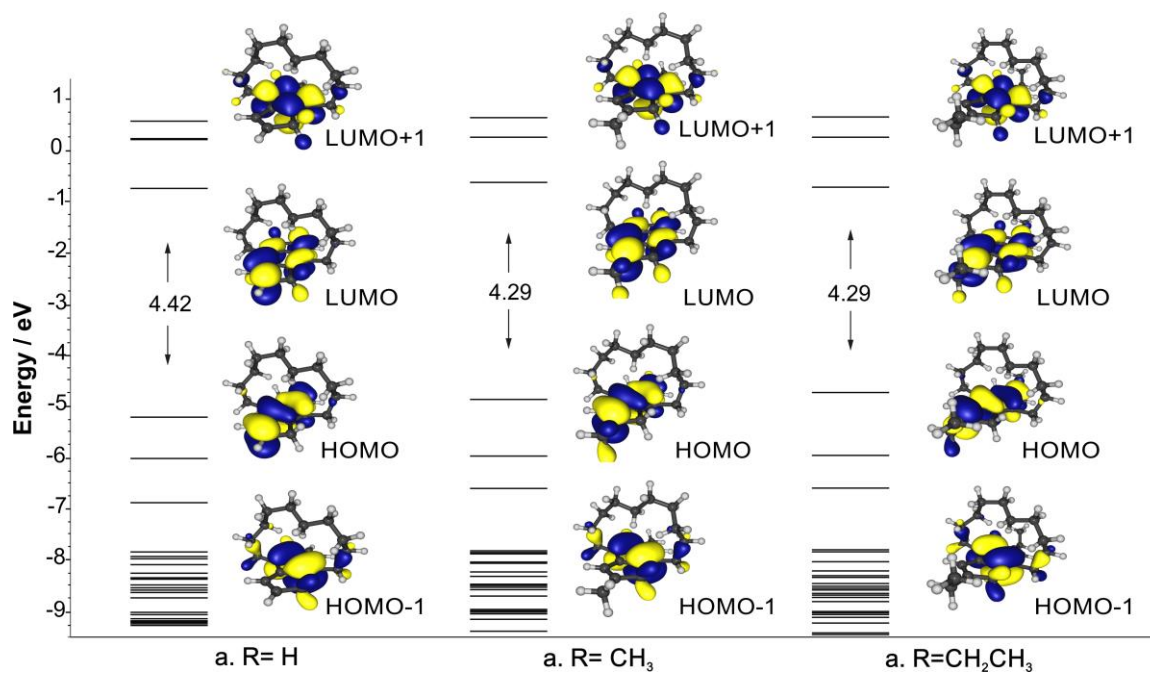


Figure S1. Structures of the studied systems. **a.** Neutral ligand.

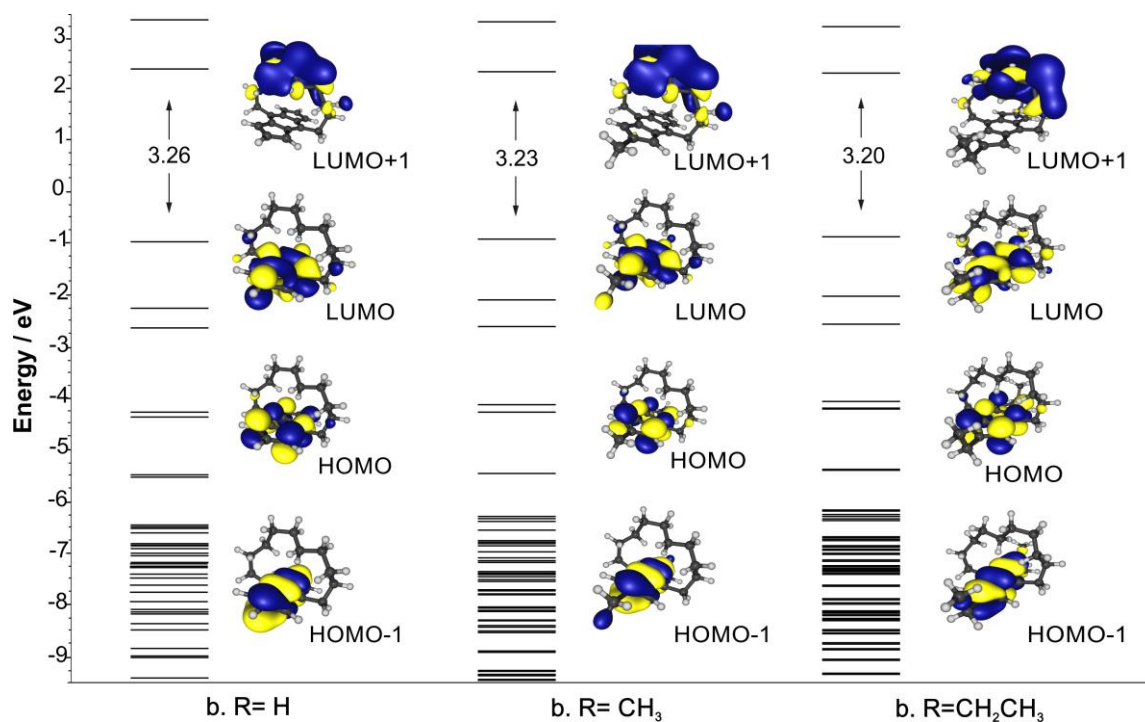


Figure S2. b. Ligand dianion.

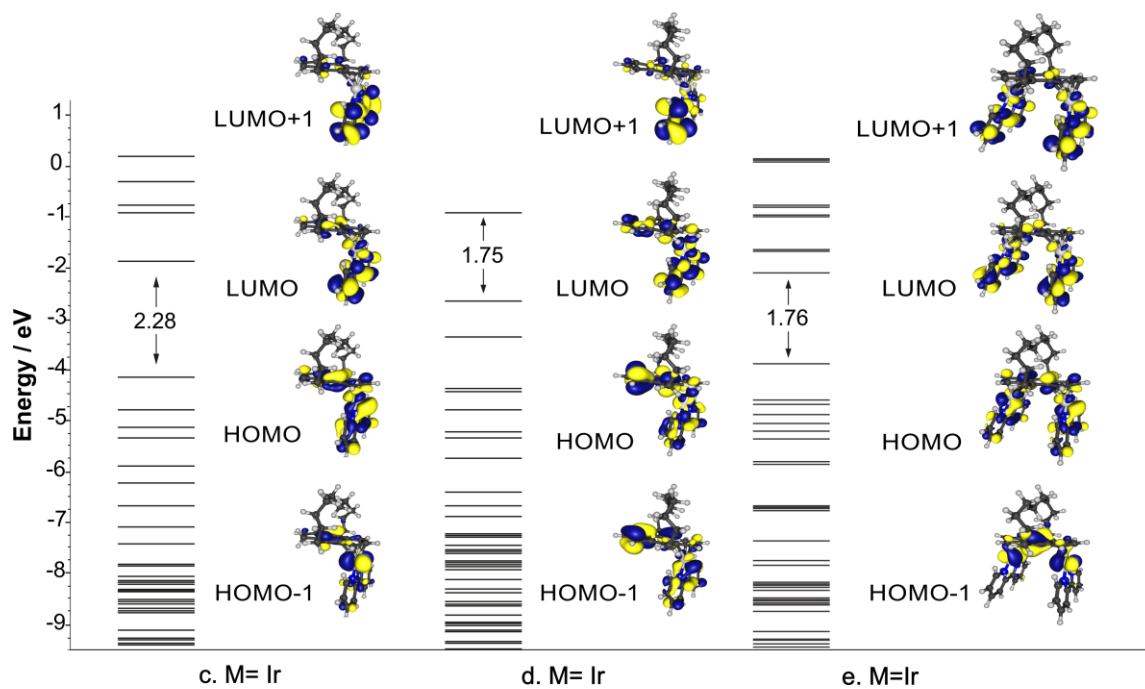


Figure S3. c. monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with M=Ir, L=bipy and R=H.

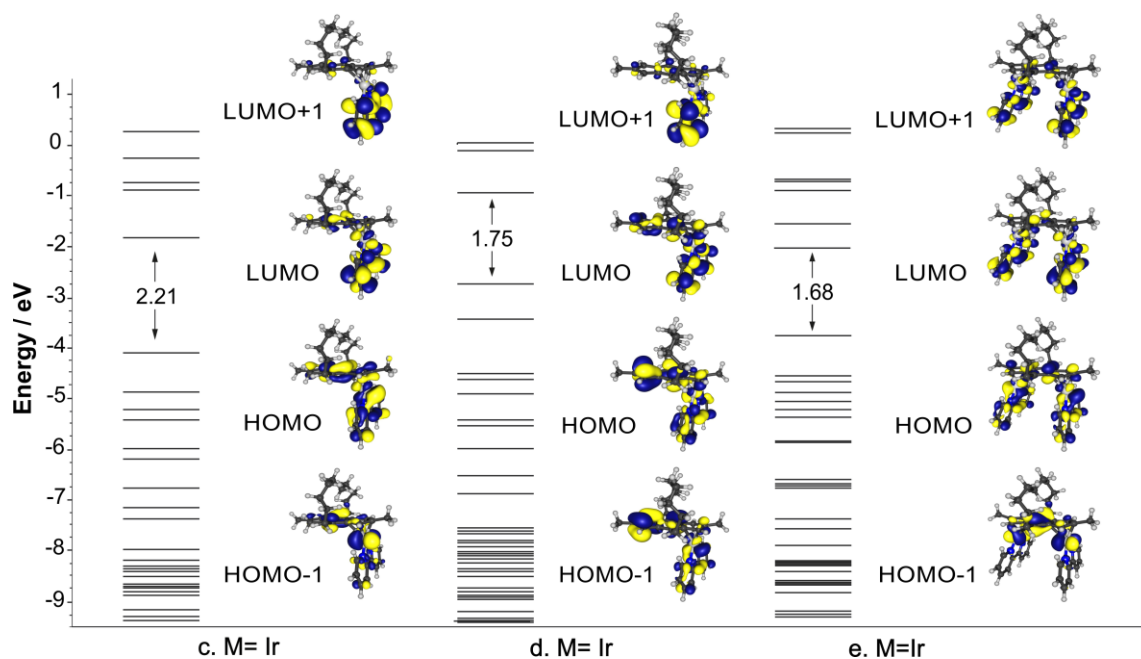


Figure S4. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with M=Ir, L=bipy and R=CH₃.

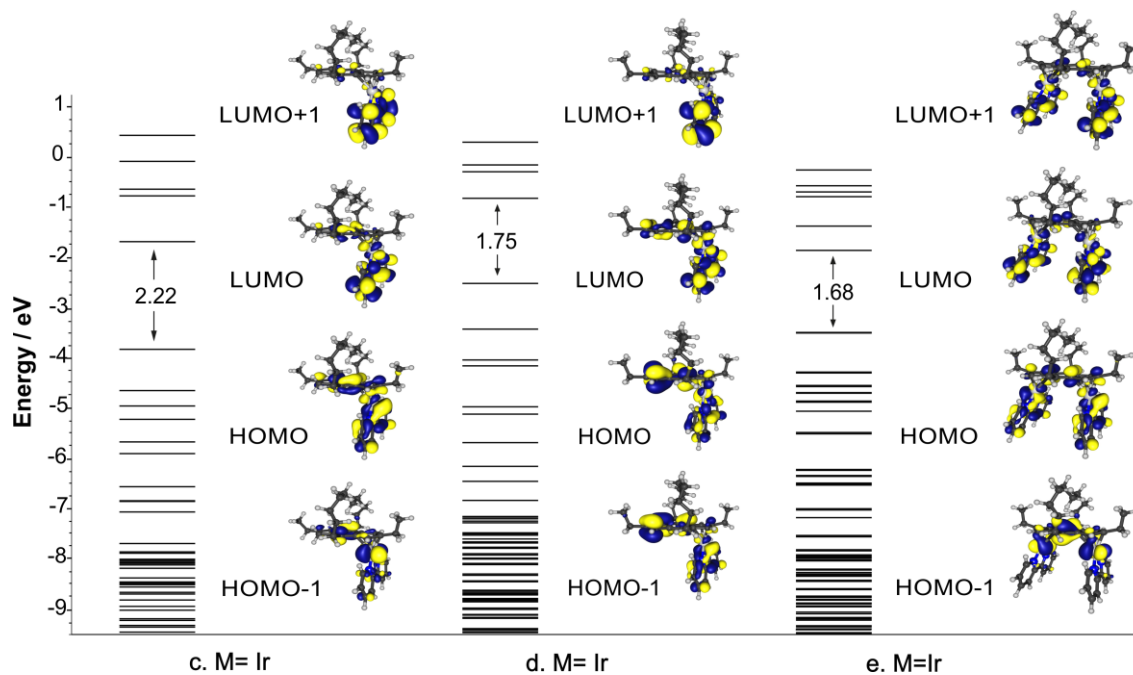


Figure S5. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with M=Ir, L=bipy and R=CH₂CH₃.

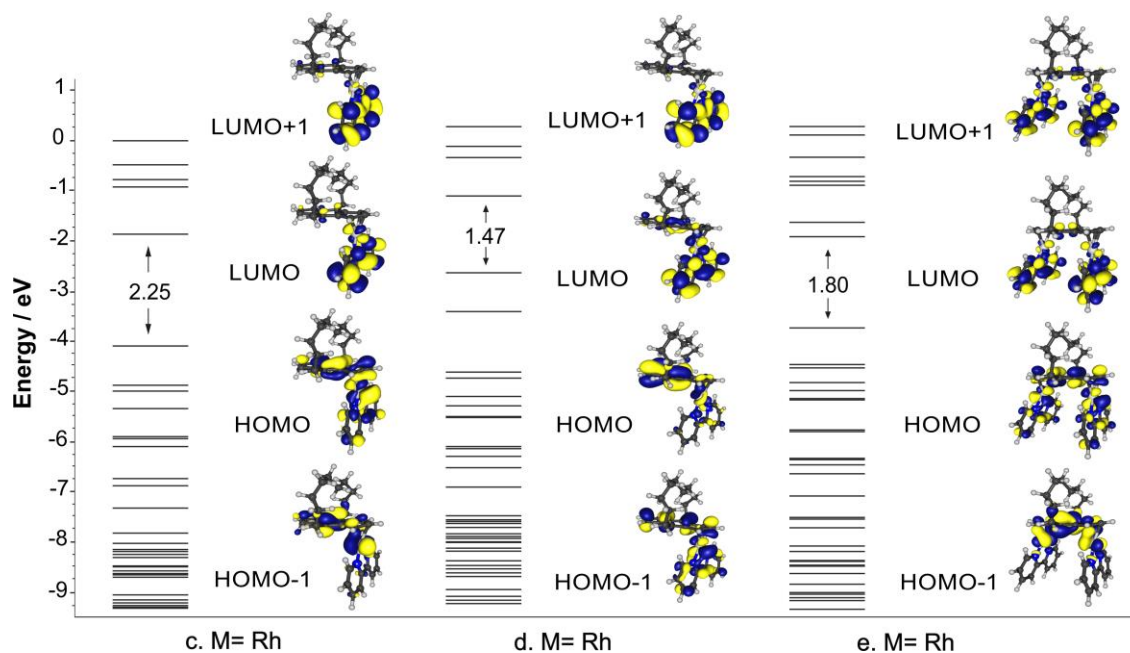


Figure S6. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with $M = \text{Rh}$, $L = \text{bipy}$ and $R = \text{H}$.

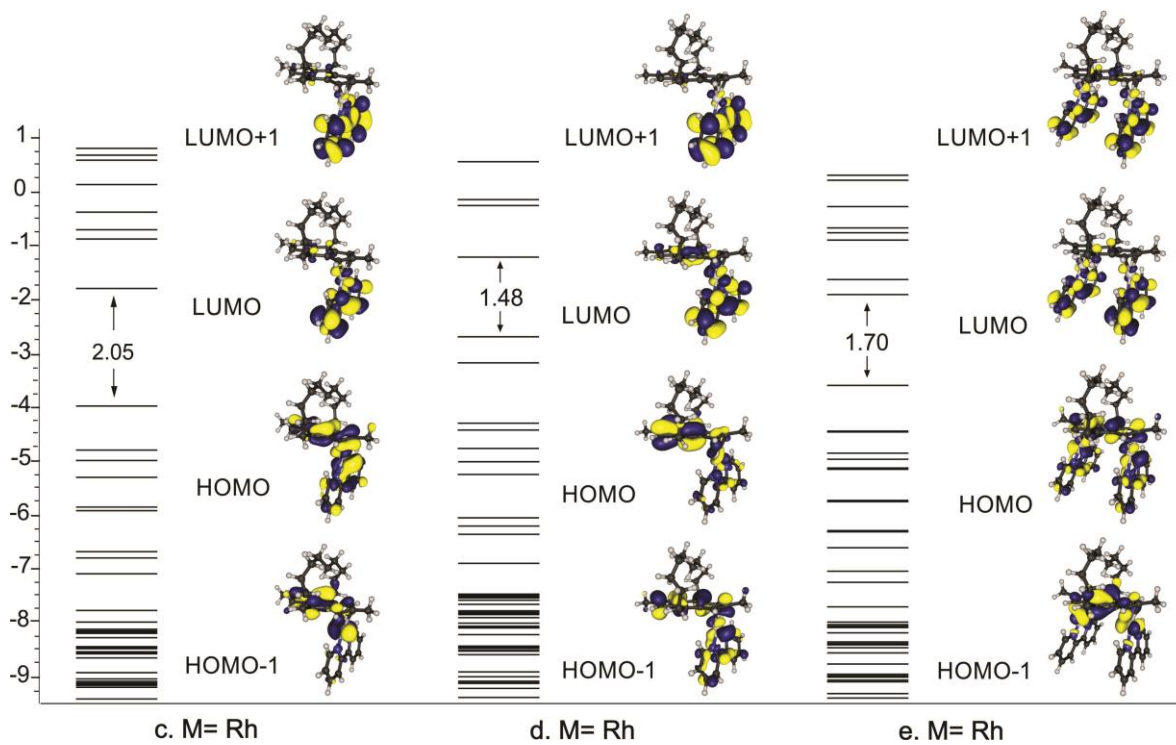


Figure S7. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with $M = \text{Rh}$, $L = \text{bipy}$ and $R = \text{CH}_3$.

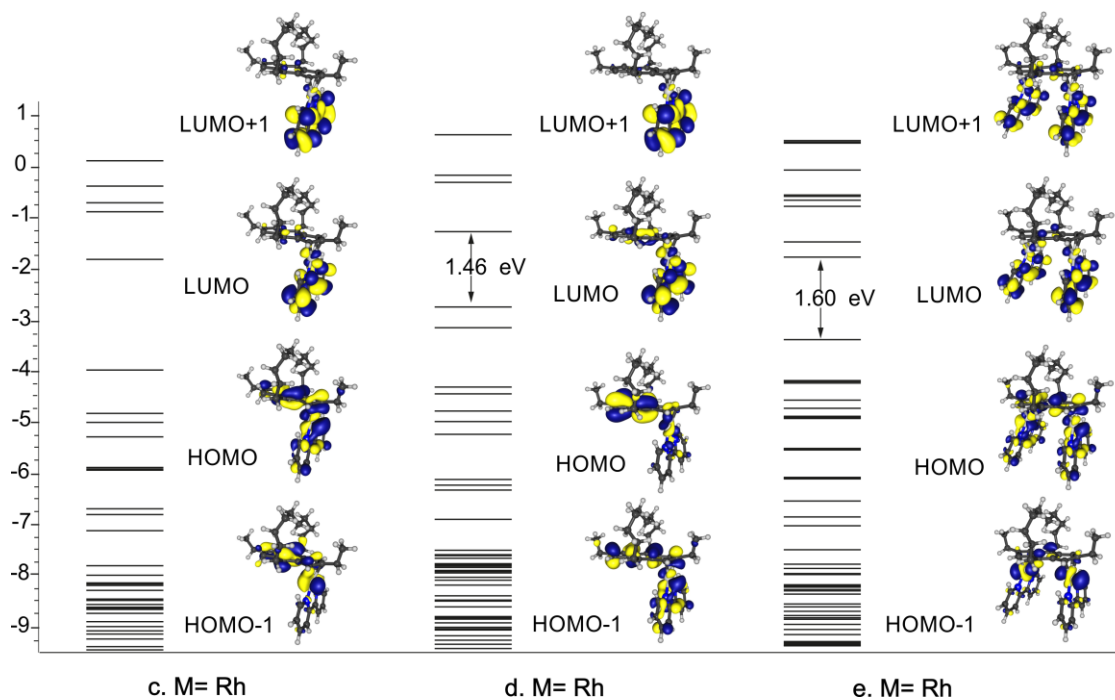


Figure S8. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with M=Rh, L=bipy and R=CH₂CH₃.

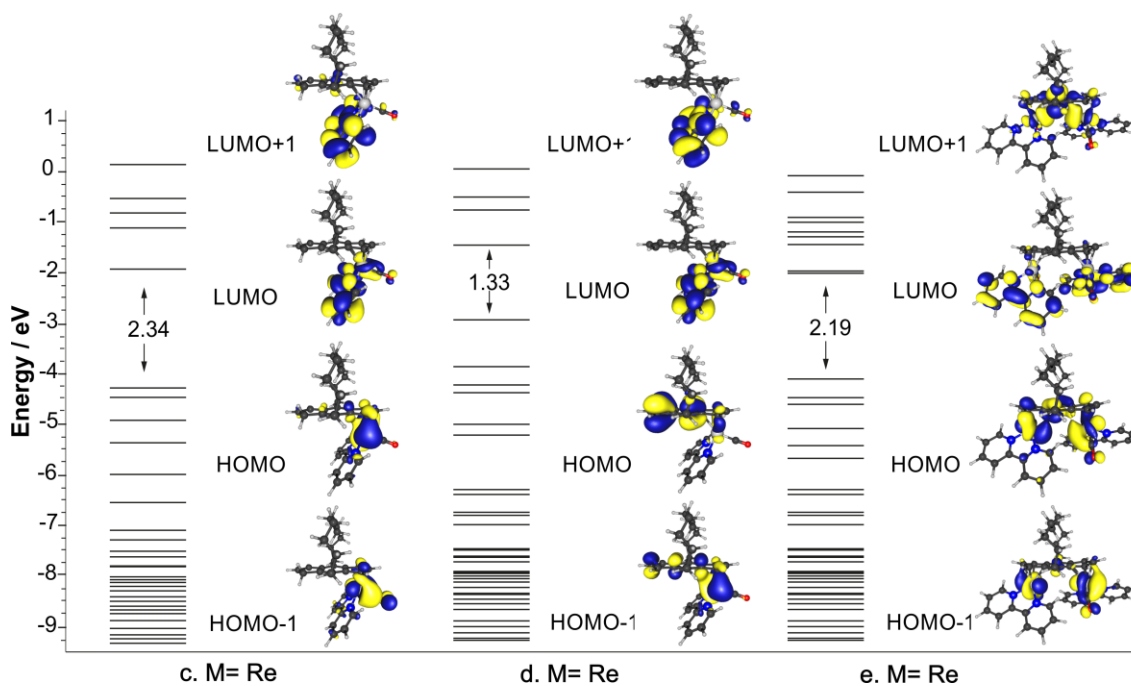


Figure S9. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with M=Re, L=bipy,CO and R=H.

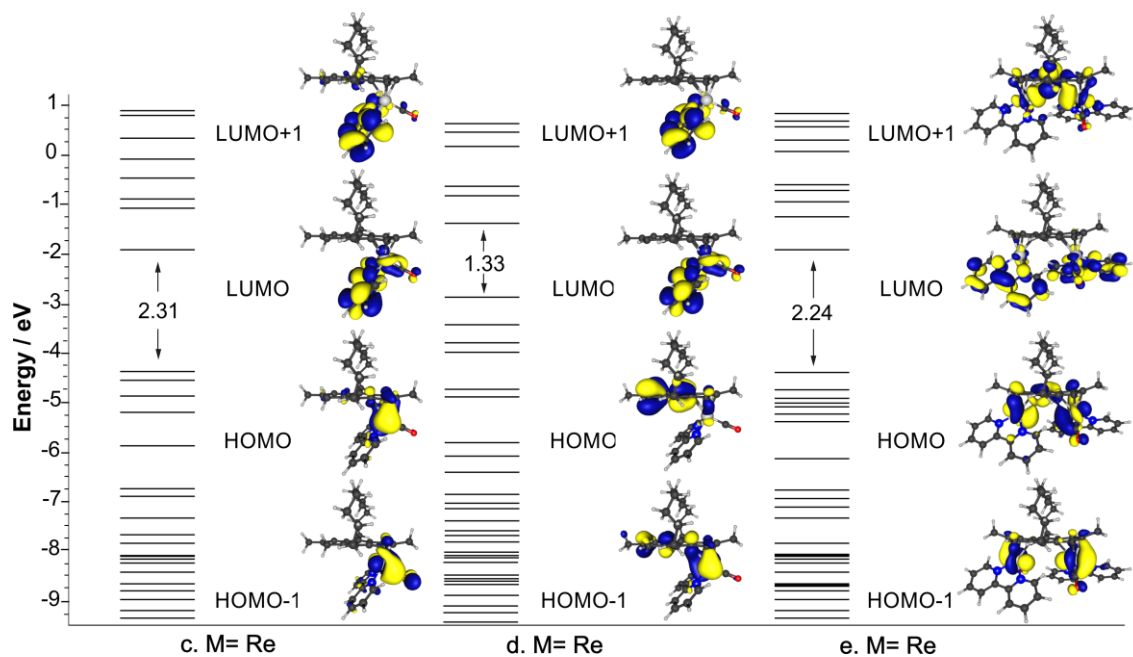


Figure S10. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with M=Re, L=bipy,CO and R=CH₃.

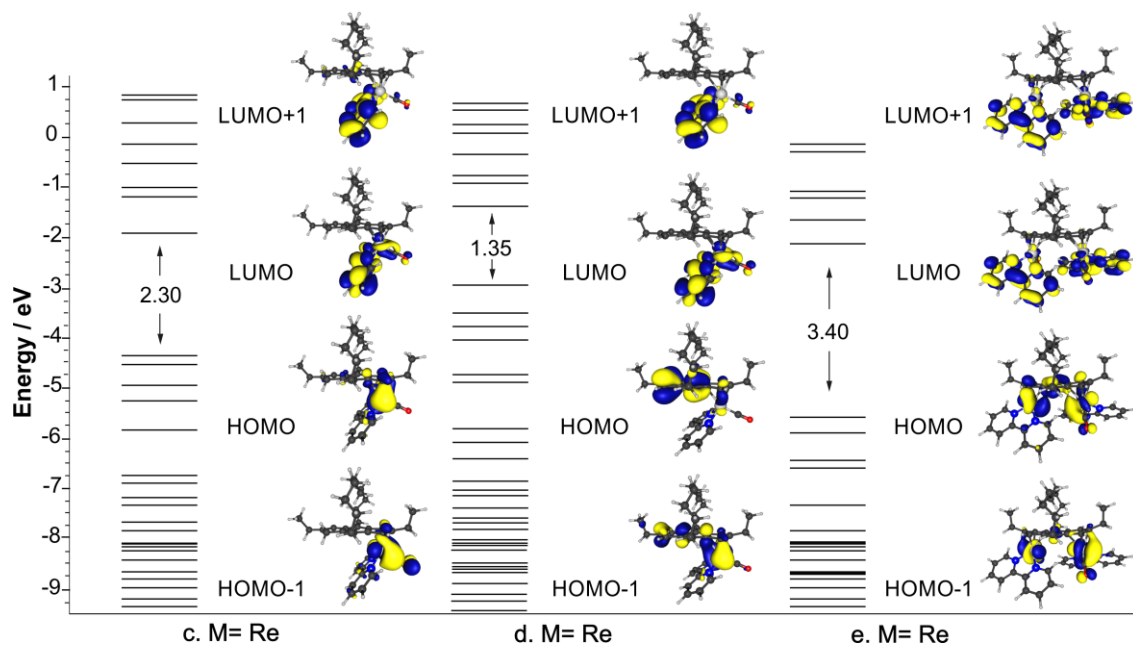


Figure S11. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with M=Re, L=bipy,CO and R=CH₂CH₃.

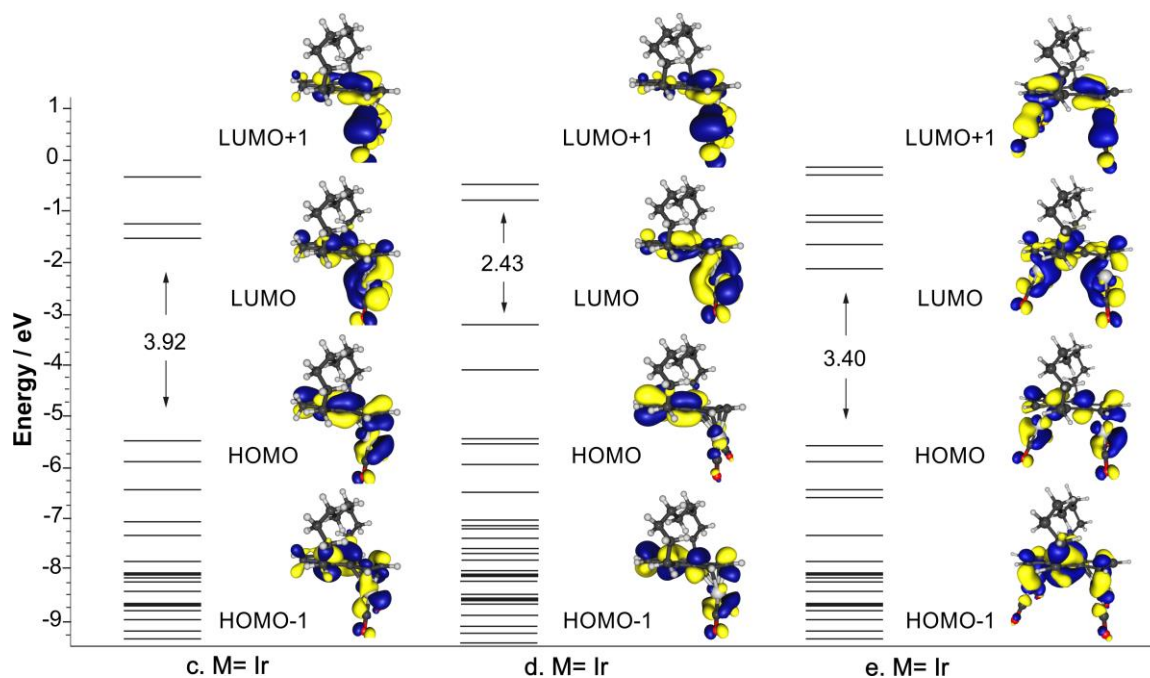


Figure S12. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with $M=Ir$, $L=(CO)_2$ and $R=H$.

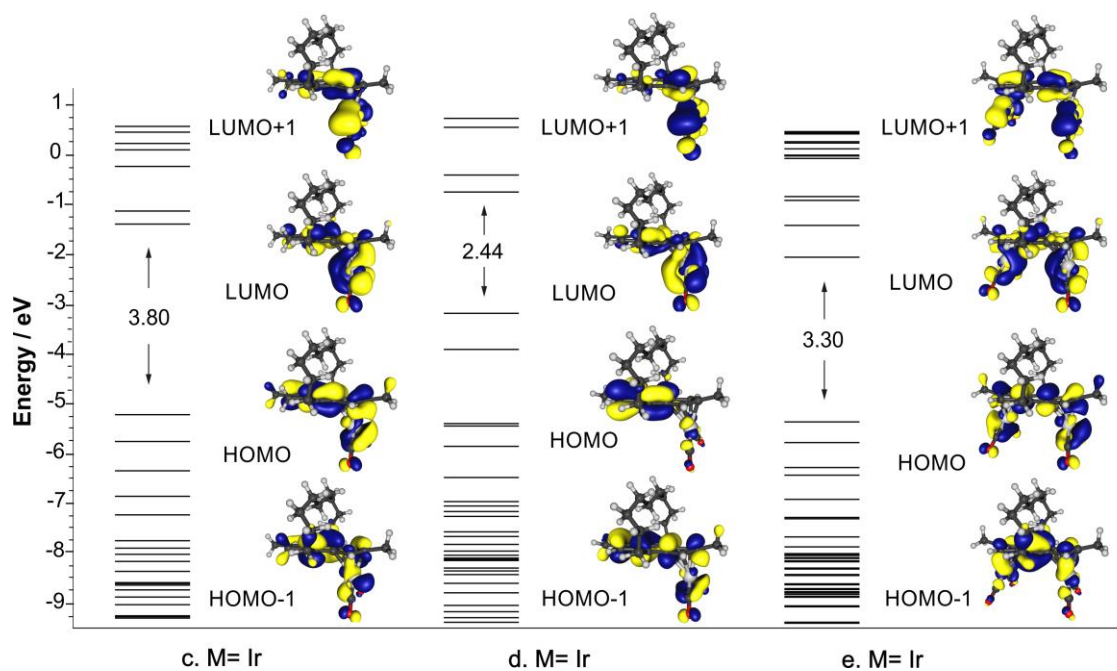


Figure S13. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with $M=Ir$, $L=(CO)_2$ and $R=CH_3$.

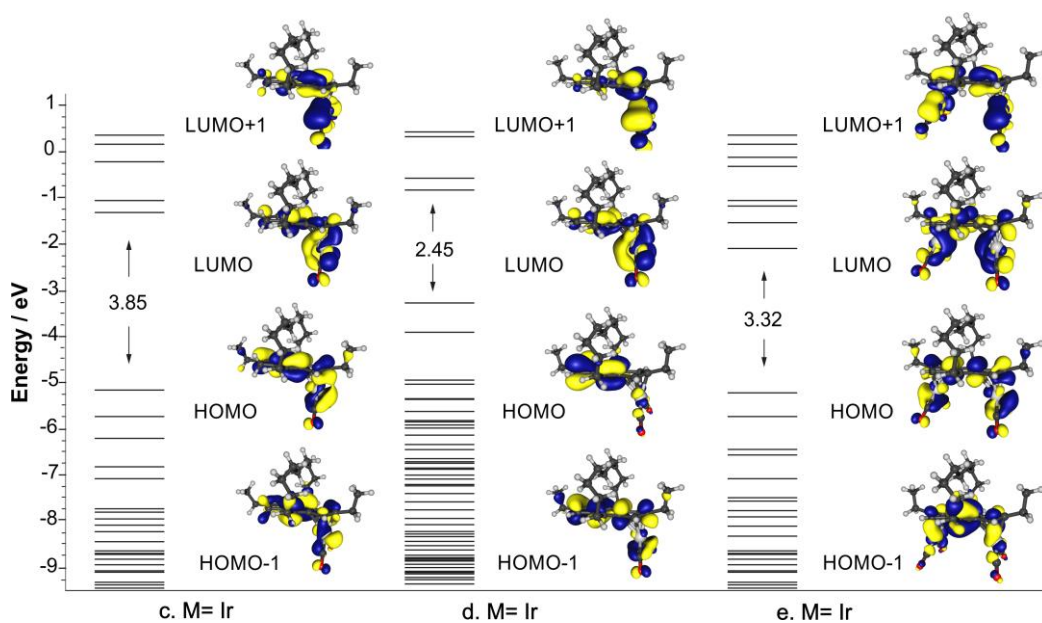


Figure S14. c. monometallic neutron, d. monometallic monoanion and e. bimetallic system with M=Ir, L=(CO)₂ and R=CH₂CH₃.

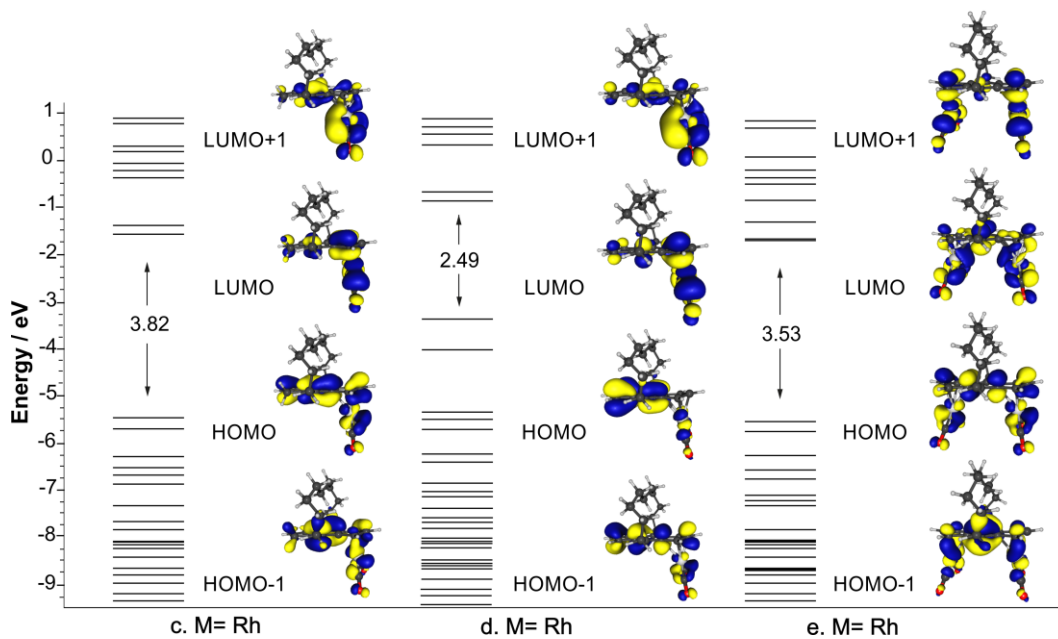


Figure S15. c. monometallic neutron, d. monometallic monoanion and e. bimetallic system with M=Rh, L=(CO)₂ and R=H.

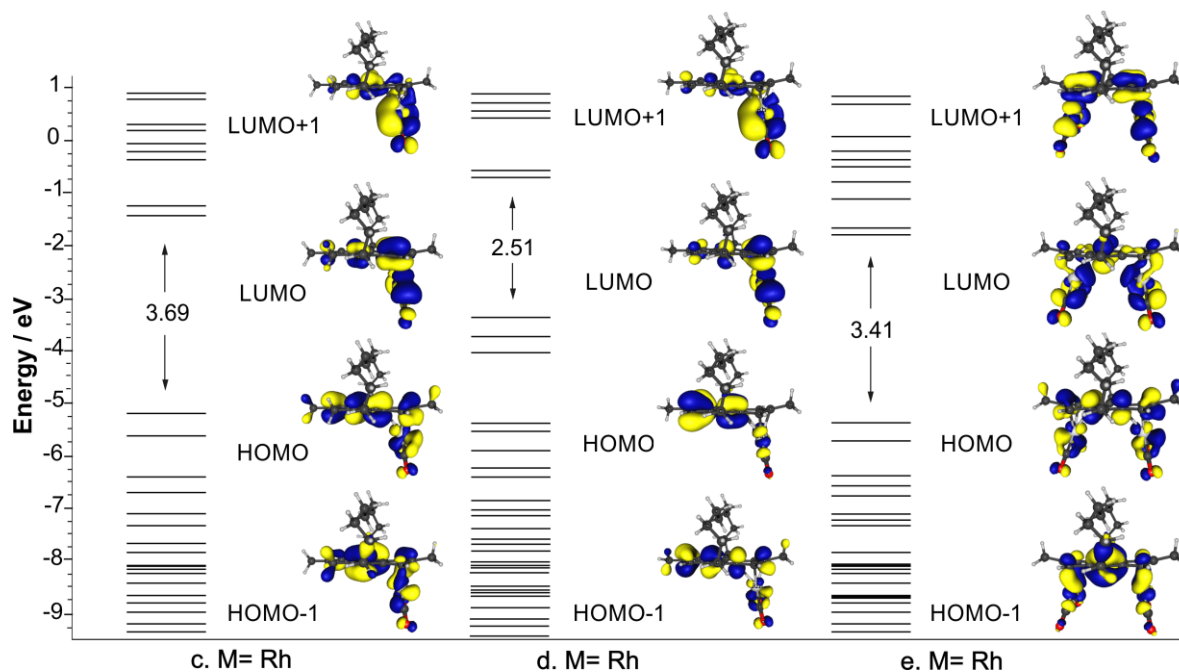


Figure S16. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with $M = \text{Rh}$, $L = (\text{CO})_2$ and $R = \text{CH}_3$.

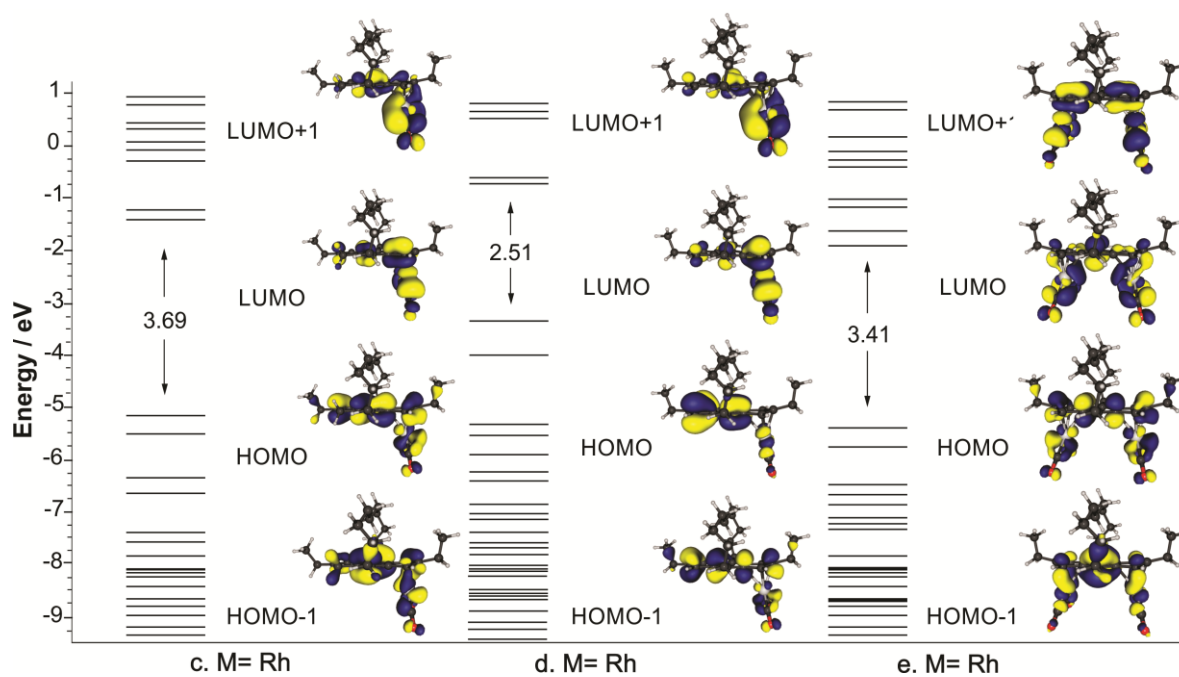


Figure S17. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with $M = \text{Rh}$, $L = (\text{CO})_2$ and $R = \text{CH}_2\text{CH}_3$.

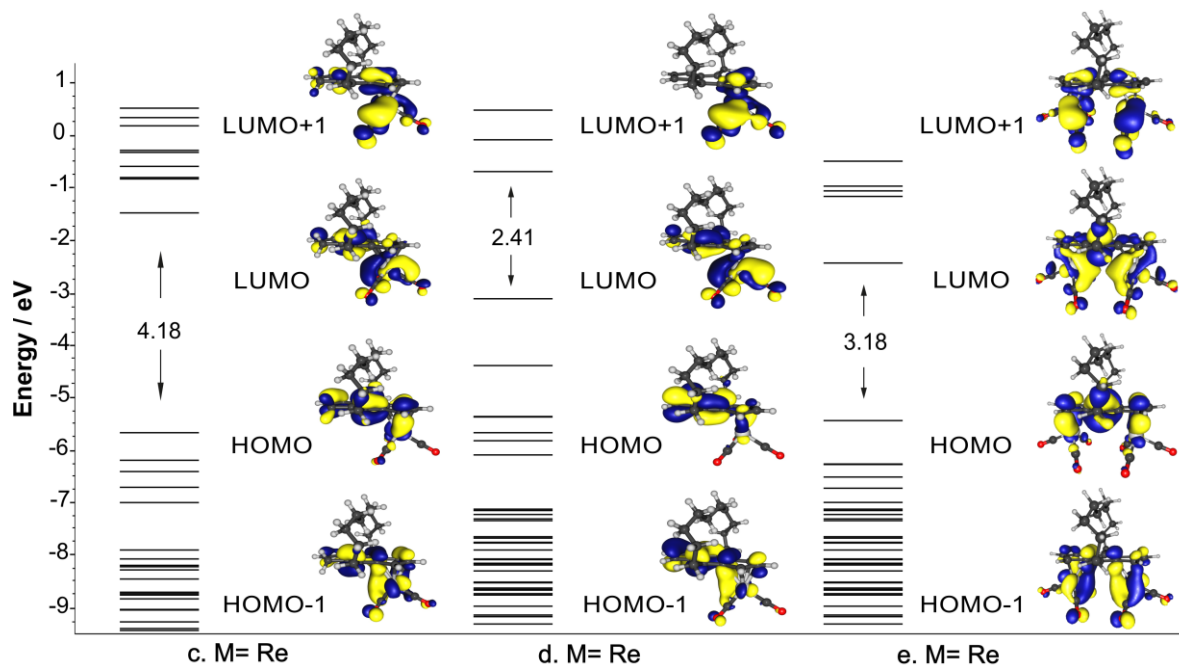


Figure S18. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with $M=Re$, $L=(CO)_3$ and $R=H$.

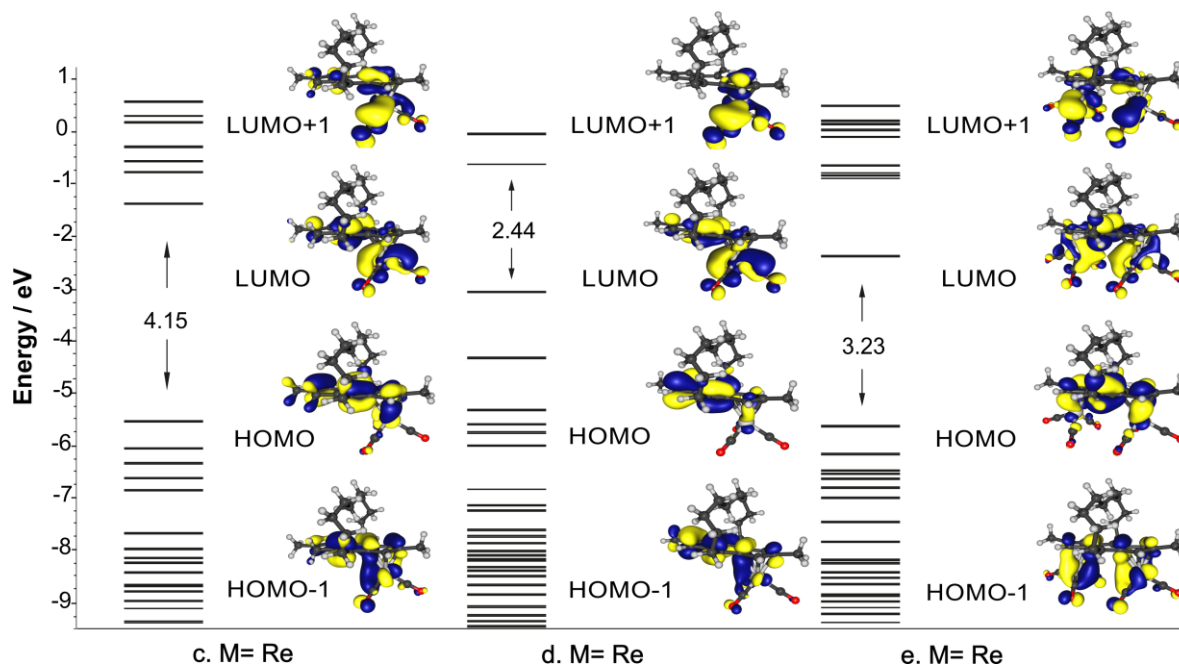


Figure S19. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with $M=Re$, $L=(CO)_3$ and $R=CH_3$.

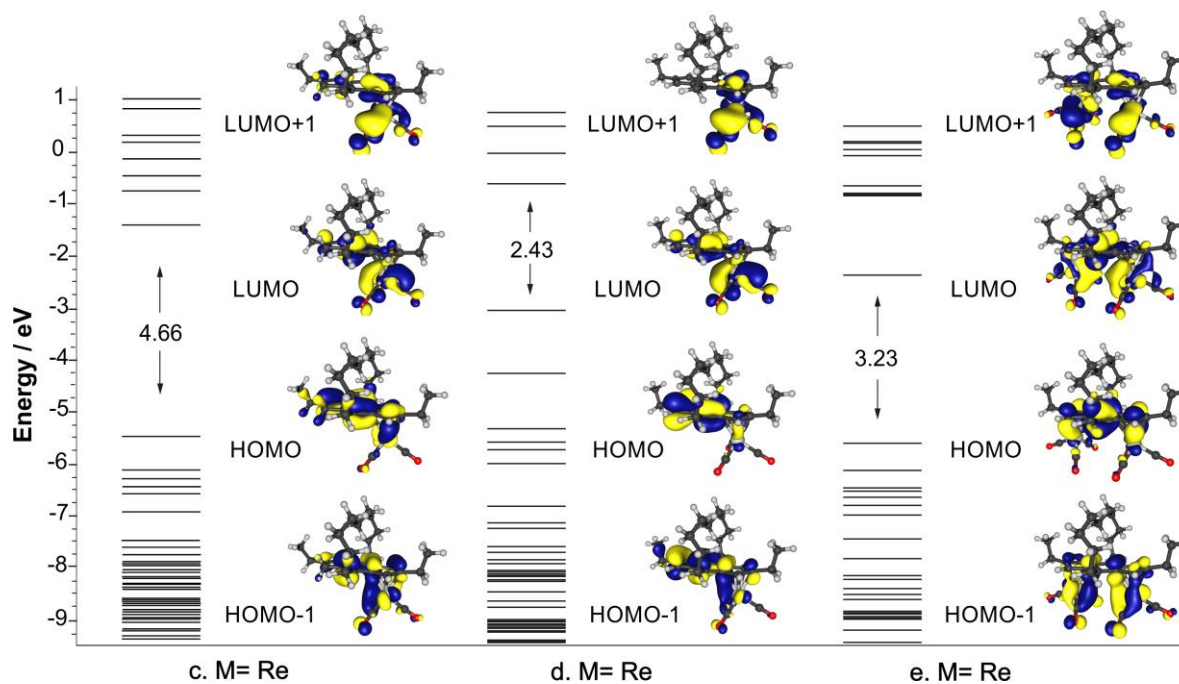


Figure S20. **c.** monometallic neutron, **d.** monometallic monoanion and **e.** bimetallic system with $M=Re$, $L=(CO)_3$ and $R=CH_2CH_3$.