

Theoretical Investigation of Electronic Structures and Properties of C₆₀-Gold Nanocontacts

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Supporting materials

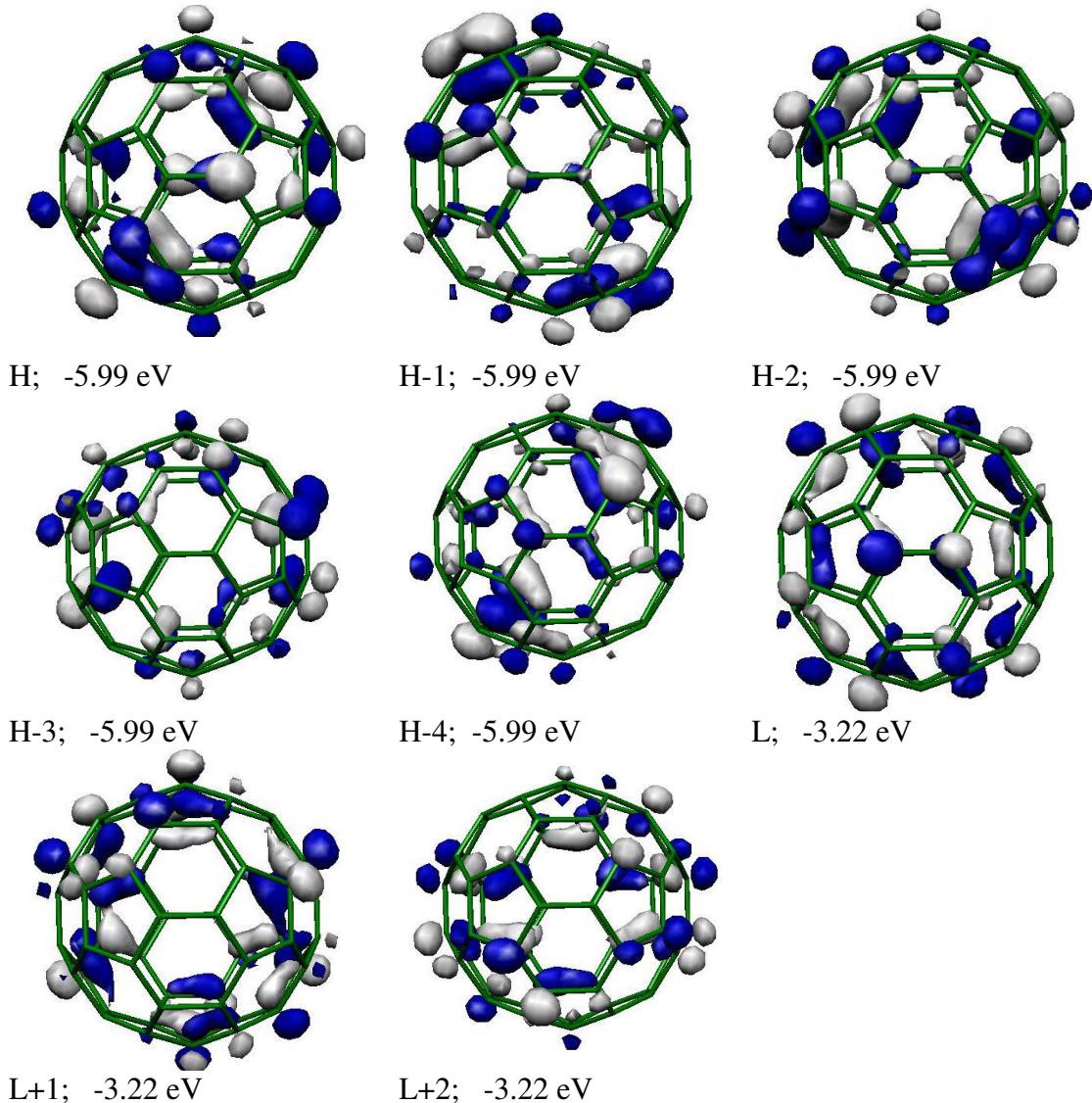


Figure S1. Frontier orbitals and orbital energies (in eV) of C₆₀ obtained at the B3LYP/6-31G(d) level.

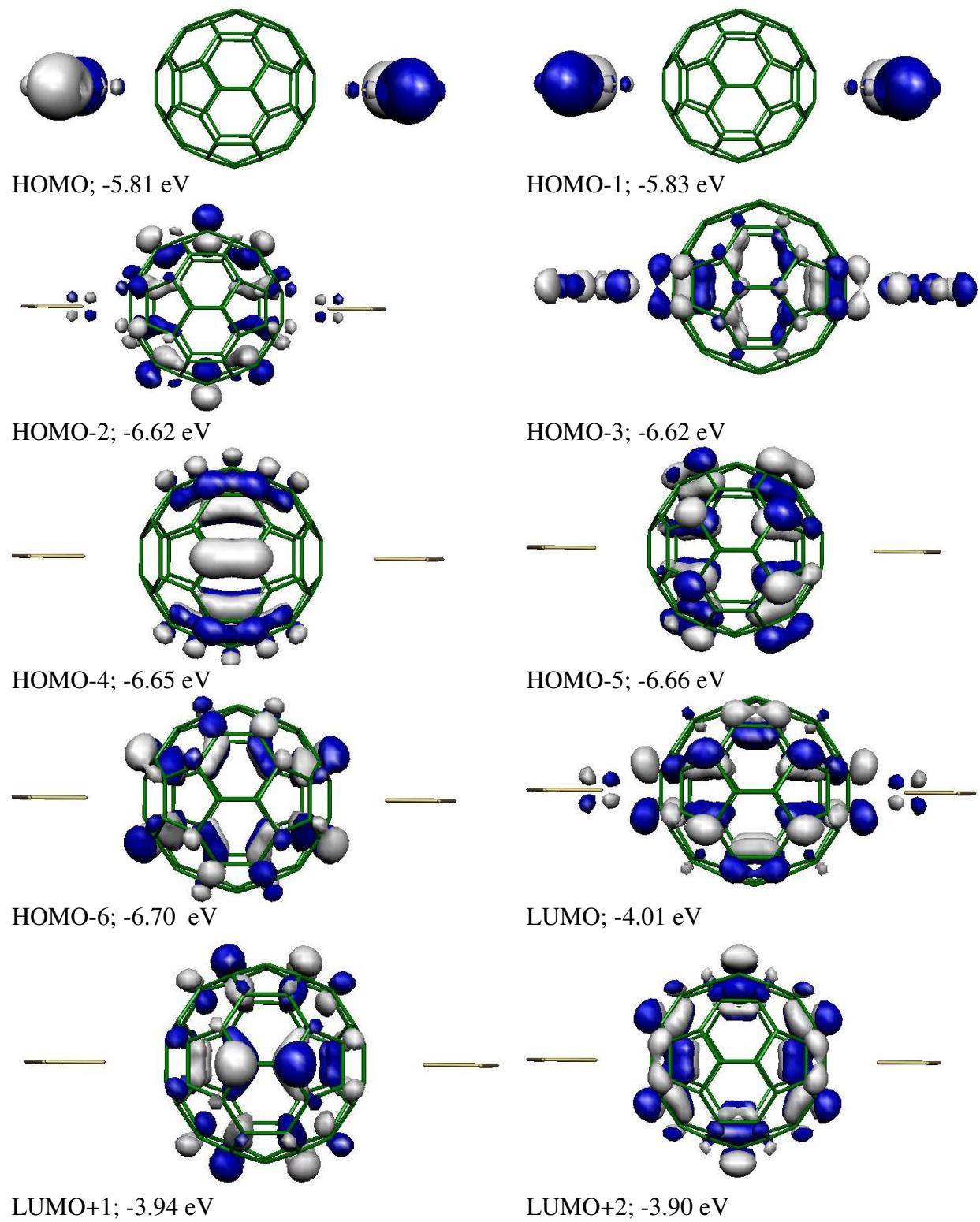


Figure S2. Frontier orbitals and orbital energies (in eV) of $\text{C}_{60}\text{-}8\text{Au}$ complex belonging to the $\eta^{2(6)}$ coordination.

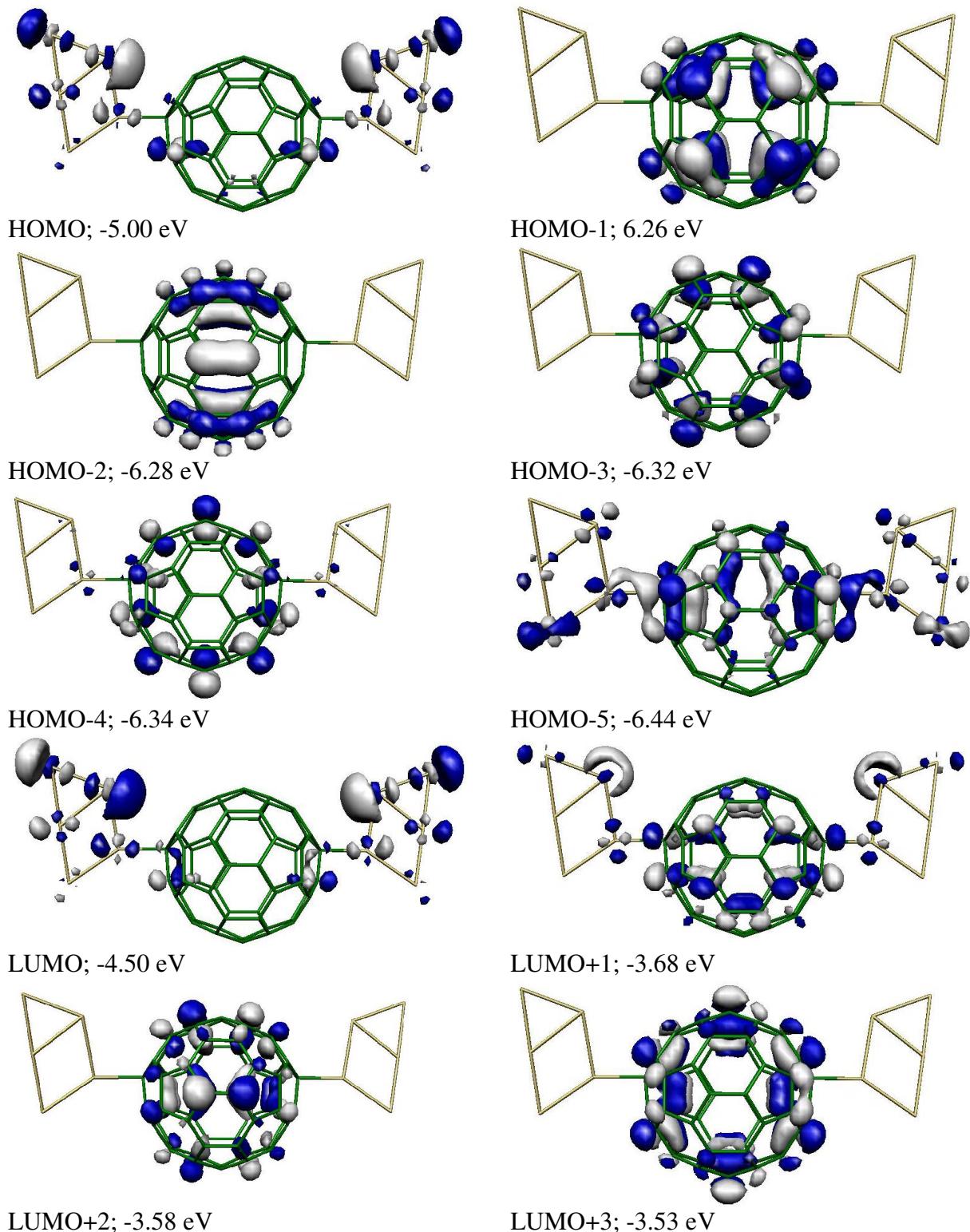
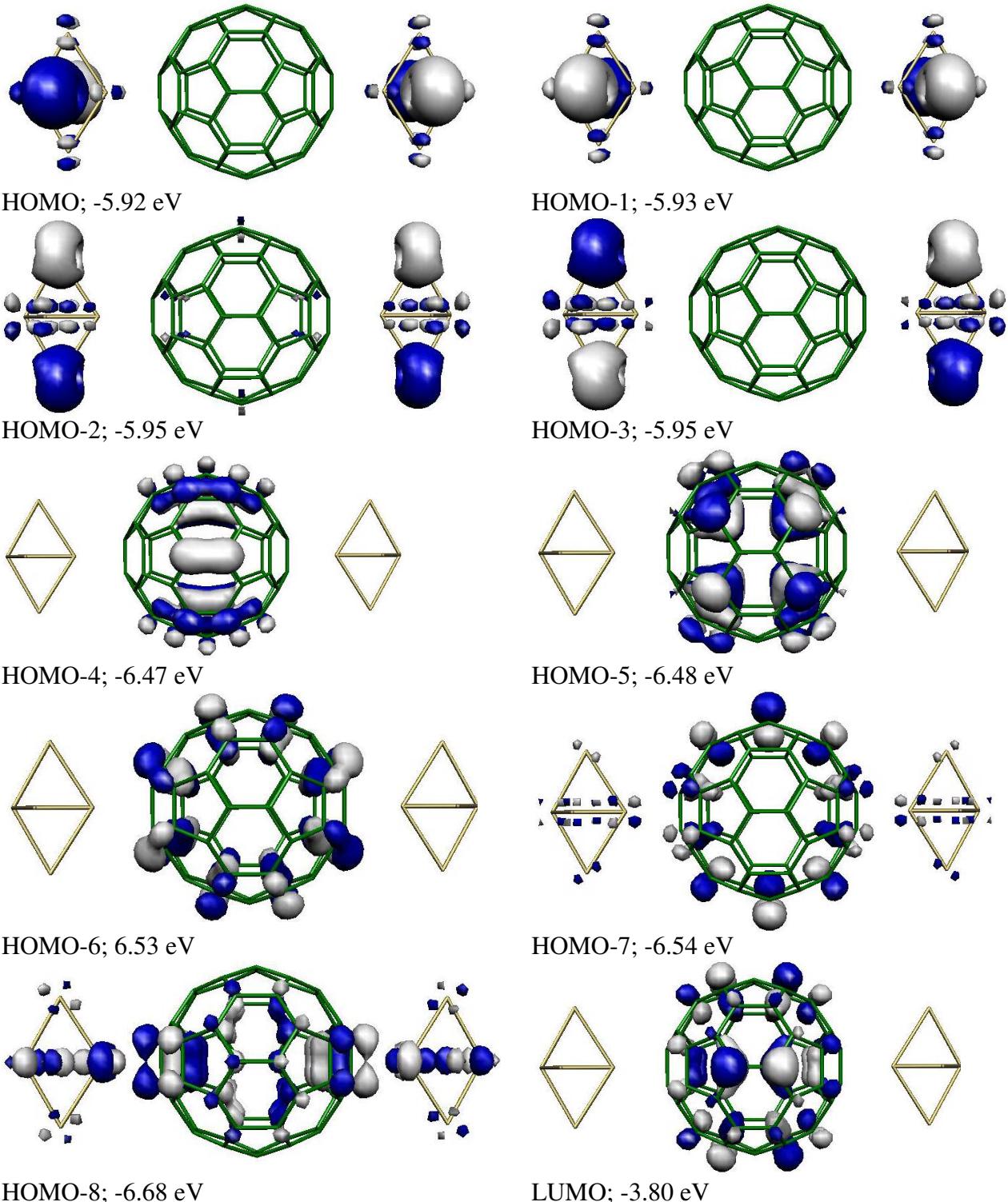


Figure S3. Frontier orbitals and orbital energies of C₆₀-10Au complex (singlet state) belonging to the $\eta^{2(6)}$ coordination.



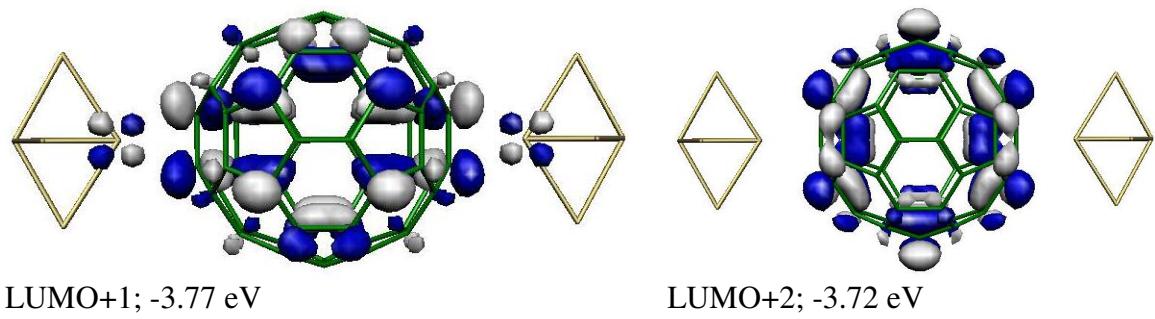


Figure S4. Frontier orbitals and orbital energies of C_{60} -12Au complex belonging to the $\eta^{2(6)}$ coordination.

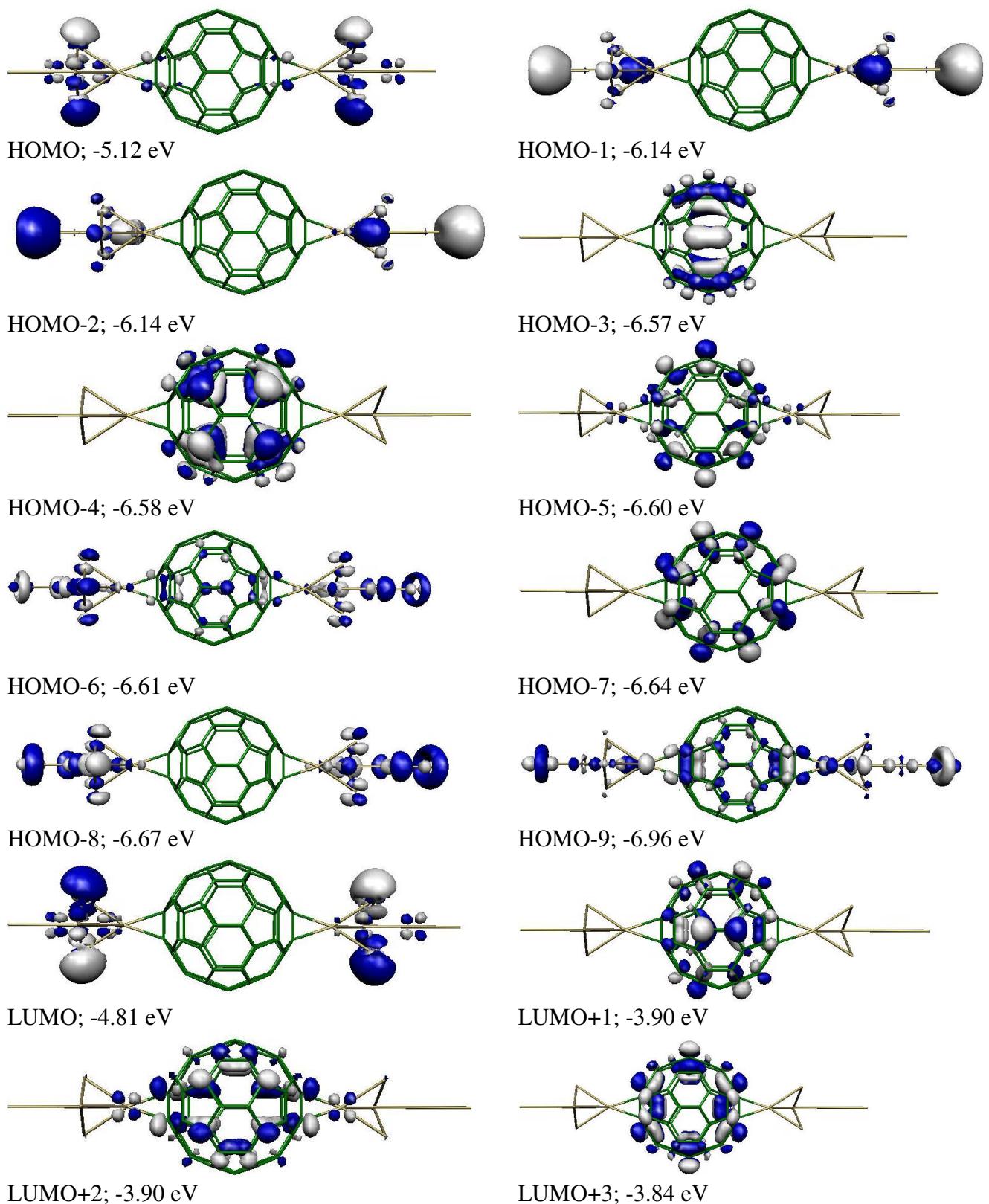


Figure S5. Frontier orbitals and orbital energies of C_{60} -14Au complex (singlet state) belonging to the $\eta^{2(6)}$ coordination.

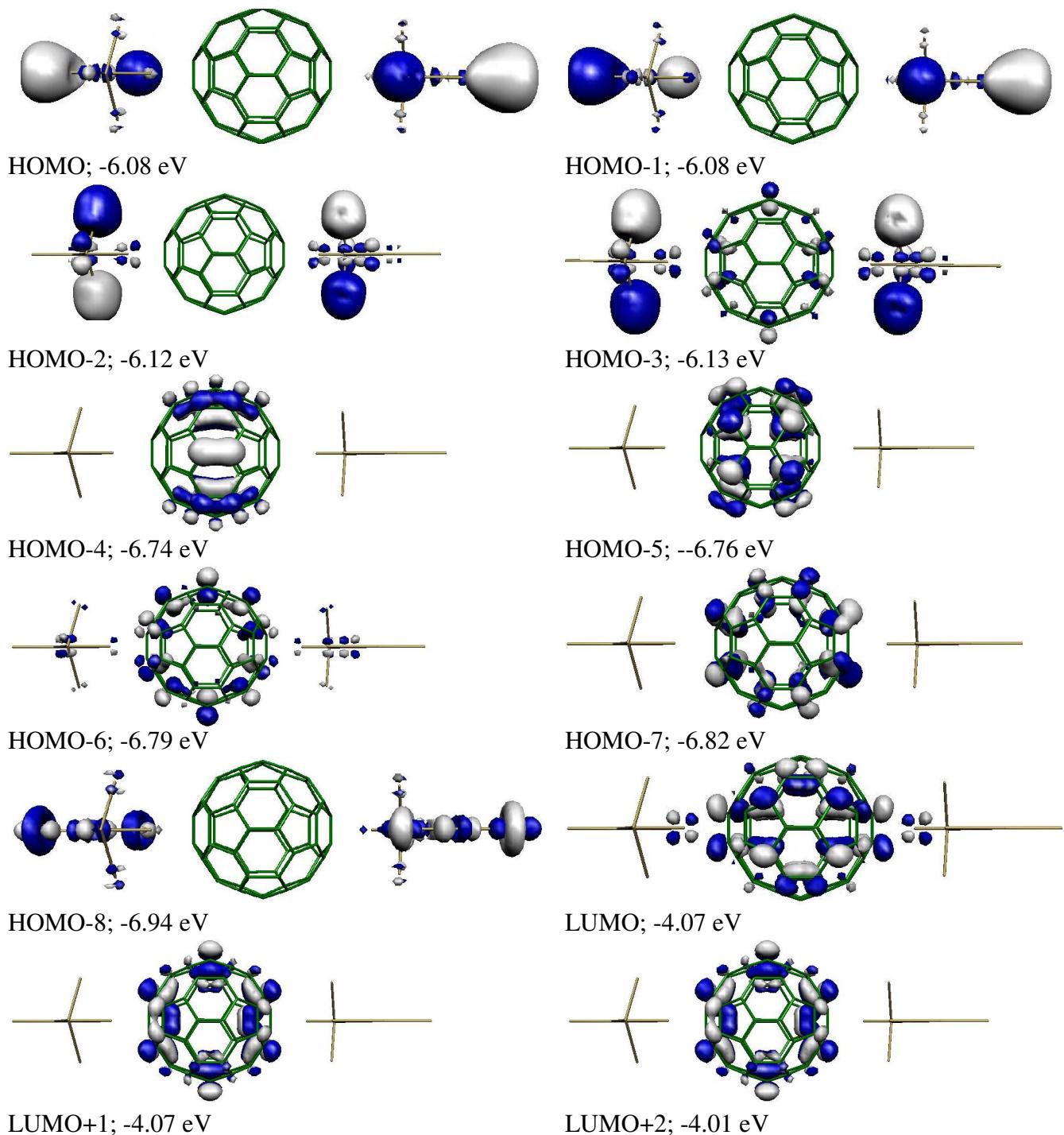


Figure S6. Frontier orbitals and orbital energies of $\text{C}_{60}\text{-}16\text{Au}$ complex belonging to the $\eta^{2(6)}$ coordination.

Complete Citation of Reference 54

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K. ; Voth, G. A. ; Salvador, P. ; Dannenberg, J. J. ; Zakrzewski, V. G. ; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision D.01. Gaussian, Inc., Wallingford CT, 2004.