Electronic Excitation Spectra of Gold Clusters: Time Dependent Density Functional Requirements

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Introduction

In recent years there has been an increased interest in the field of computational chemistry as various methods such as Densitfy Functional Theory have provided an economical way to compute various molecular level phenomenon including otical spectras.

Gold is a popular metal found in many electronic devices and jewlrey because of its various properties. Iterestingly gold behaves differently at a molecular level when compared to its bulk state. In bulk gold has a nice golden colour but at a molecular level it appears reddish [1].

Computationally gold is challenging due to its location in the periodic table. Because of its location it is necessary to include relativicstic affects and use an effective core potential [4].

Of interest in this study are the Desity Functional Theory functionals which provide the most accurate absorption, emmission, and circular dicromism results for gold clusters.

Methods

All calculations were done using Gaussian[2] with the LANL2DZ effective core potential / basis set to ensure that relativistics affects were included.

Primary calculations methods include:

- CIS
- EOMCCSD
- TD-HF
- TD-DFT with the following set of exchange and correlation functionals

Type	Exchange / Correlation Functional Pair		
Traditional		BP86	PBE
Hybrid	B3LYP	B3P86	
Long Range Corrected	CAM-B3LYP	LC- BP86	LC-PBE

Table 1: TD-DFT Exchange and Correlation Functional Pairs used

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Results

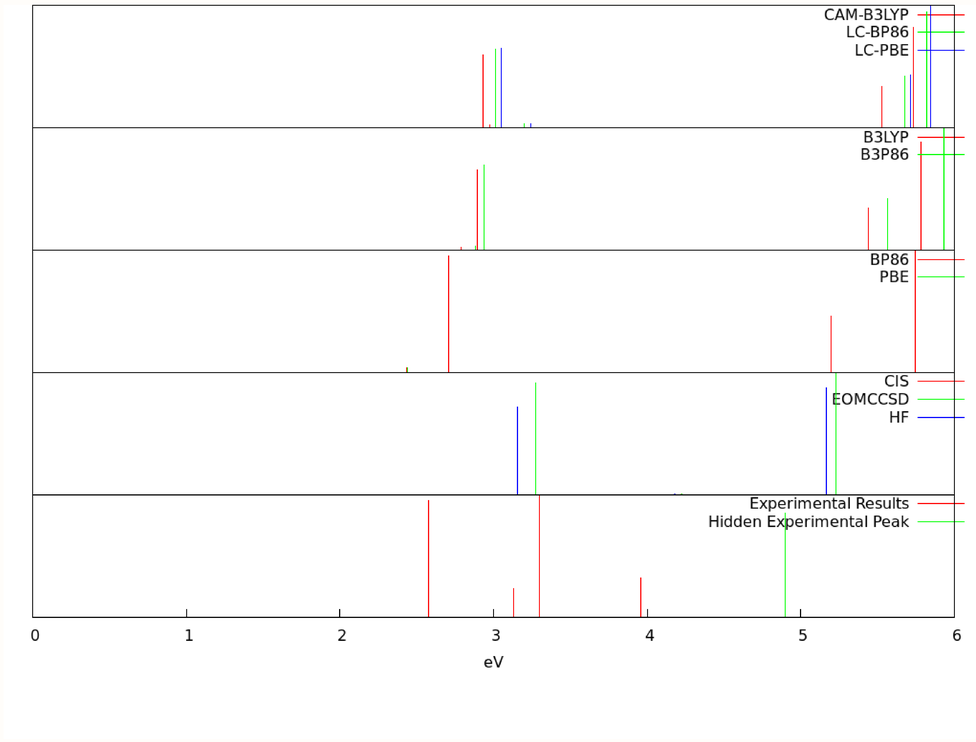

Figure 1: Absorption Spectrum of Au_2 as computed by various methods

Ongoing and Future Work

Calculating the absorption, emmission and circular dicromism spectrum of:

- Additional gold geometries with various bondlengths
- Bent linear gold molecules

Using this knowledge we can determine the optimal TD-DFT functional(s) to use with determining the spectra of novel gold helicies[3].

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