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Density Functional Calculation of Metal Dithizonates

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<p>Understanding molecular dynamics on potential energy surfaces has been at the heart of ultrafast transient absorption in the recent years [Philipp K, etal., 2005],[Karel G, etal., 2008]. Based on the on-going experiment at our ultrafast laboratory, we ran density functional calculations on metal dithizonates, starting with their kernel molecule, formaldimine, to validate what we observe experimentally. This we treated in terms of ground state energy, absorption spectrum, vibrational frequency and potential energy surface using two different softwares: Amsterdam Density Functional (ADF) and Gausian(09). The overall results show that B3LYP functional combined with CEP-31G basis set gave the closest results to the experimentally observed data.

Level (Hons, MSc,
   PhD, other)?

MSc

Consider for a student
   award (Yes / No)?

Yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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