Relativistic Coupled Cluster Theory

Avijit Shee, University of Michigan

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7th Floor Lounge, 711 Havemeyer

I will provide a brief background of relativistic electronic structure theory- the choice of Hamiltonian and mean field to electron correlation theories. A major deterrent of applying established electron correlation methods is the computational cost. I will show how the use of relativistic symmetry can help to some extent. The importance of relativistic electronic structure theory is more apparent when applied to molecular properties, mostly when spin-orbit coupling plays an important role in it. I will discuss how that is done in DIRAC quantum chemistry package at the coupled cluster level. Finally, if time permits I will discuss open-shell correlation treatment via fully relativistic equations of motion coupled cluster (EOMCC) theory.


Plenty of pizza will be provided.