Calculation of response properties using Extended Coupled Cluster Method

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Extended Coupled Cluster (ECC) Method is used for calculation of response properties. Due to double linking nature of the functional, there are no disconnected terms present in the calculation of energy and energy derivatives and the series gets naturally terminated. Double linked nature of the functional ensures that we always have size extensive properties. ECC being variational is best suited for the property calculations.

Spectroscopic properties such as IR intensities, Raman intensities and viberational frequencies are calculated using ECC approach. We have used semi-numerical approach for these calculations[1] . IR and Raman intensities are the derivatives of energy with respect to electric field and geometric perturbation while, viberational frequencies are the derivatives of energy with respect to geometry. Recently, the analytic ECC approach has been applied for evaluating dipole-quadrupole polarizability [2]. Dipole-quadrupole polarizability, is the second derivative of energy with respect to field and field gradient.

[1] S. P. Joshi, A. K. Dutta, S. Pal, N. Vaval Chem. Phys. (2012), 403, 25-32.
[2] S. P. Joshi, N. Vaval Chem. Phys. Lett. (2013), 568-569, 170-175