Evaluating the convergence rate of the finite size effects in the thermodynamic limit of connectivity-twist-averaged coupled cluster calculations in the uniform electron gas

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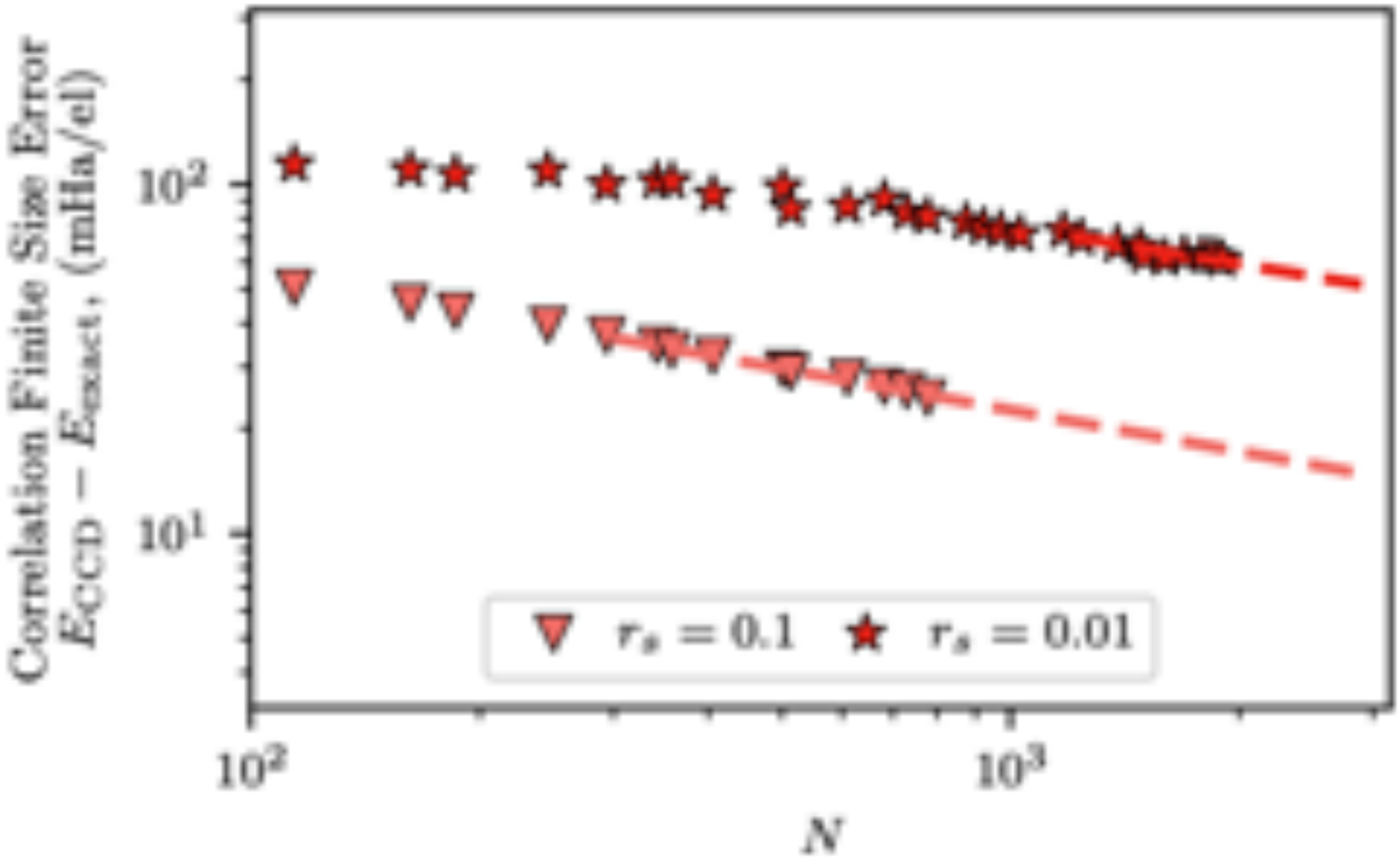
Virtual Workshop on Recent Developments in Electronic Structure Methods, UC Merced



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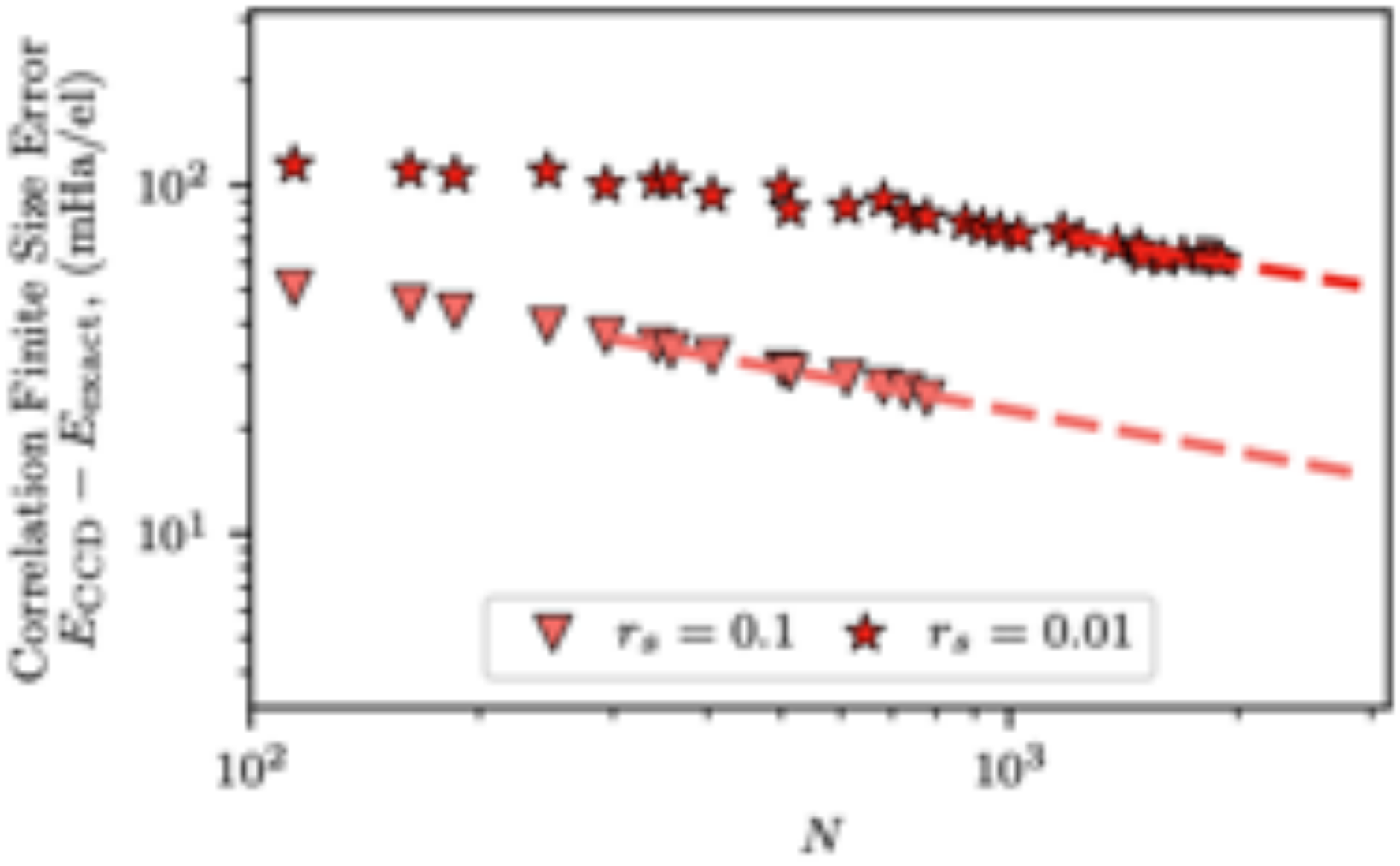
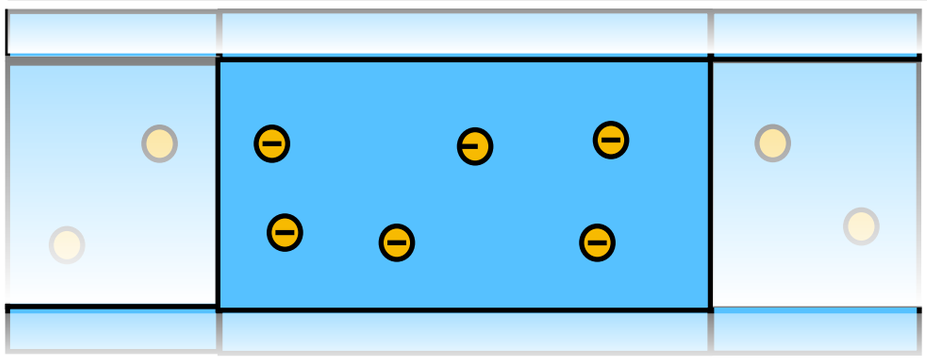
We recently found a new power law for plane waves in the coupled cluster correlation energy approach to the TDL using a cost saving twist averaging scheme in the UEG

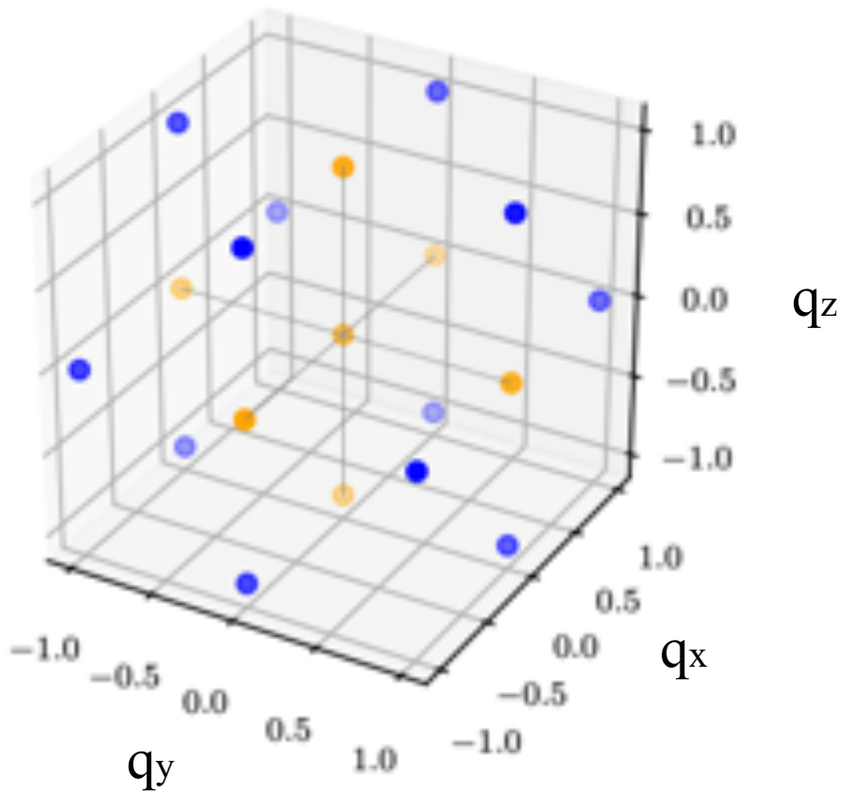


We work with the 3D uniform electron gas model system for our coupled cluster doubles calculations:

UEG



FT



CCD

$$\Psi_{CCD} = e^{\hat{T}_2}\Psi_{\mathrm{HF}}$$

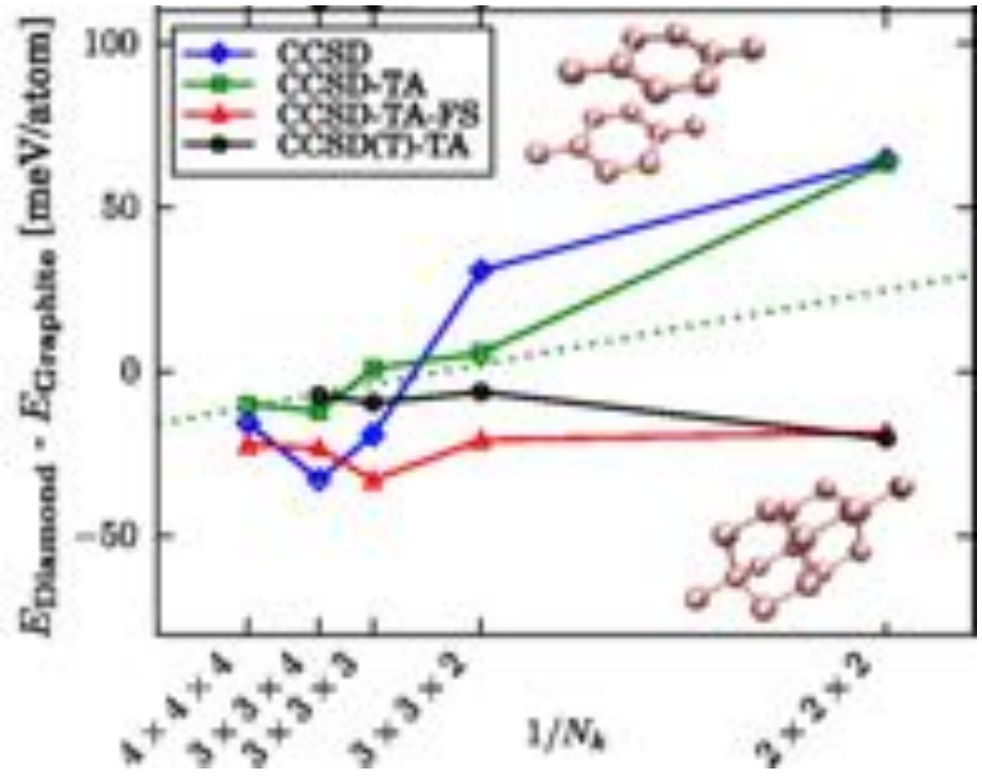
$$E_{CCD} = \langle \Psi_{\mathrm{HF}} | \hat{H} | \Psi_{CCD} \rangle$$

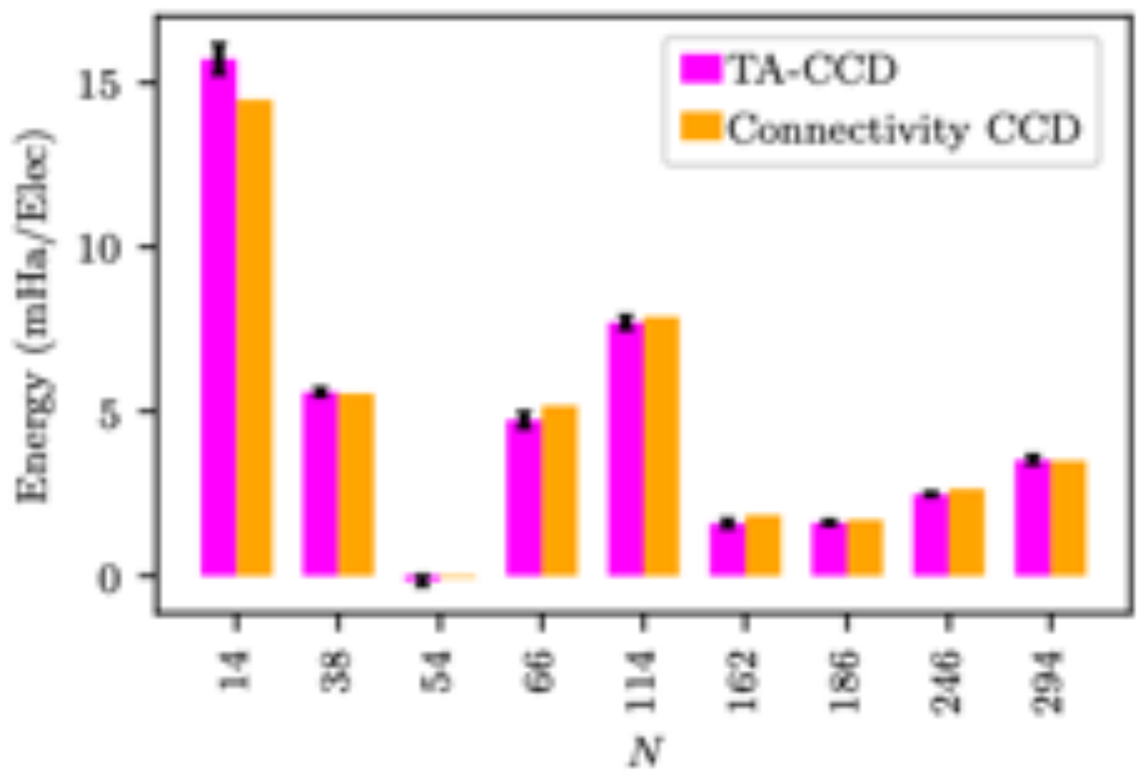
$$E_{CCD} = E_{HF} + E_{corr}$$

$$E_{corr} = \frac{1}{2} \sum_{ijab} t_{ijab} \overline{v}_{ijab}$$

***Calculations run on supercells**

Twist-averaging is used to reduced some the finite size effects in solids
We recently developed a cost saving twist averaging scheme in the 3D-UEG that allows us to go out to system sizes up to 2042 electrons

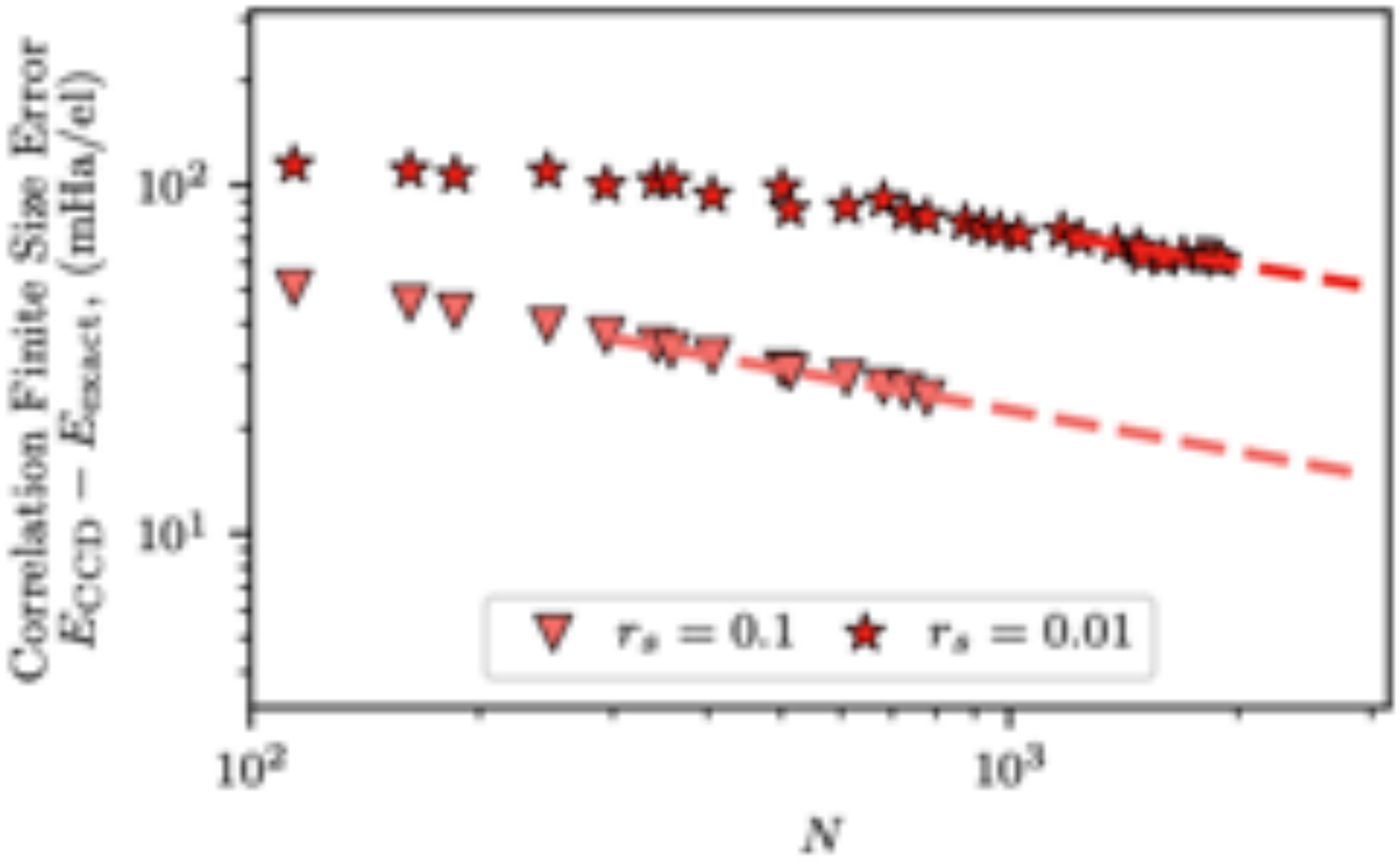




T. Gruber, K. Liao, T. Tsatsoulis, F. Hummel, and A. Grüneis, *Phys. Rev. X*, **8,** 021043 (2018)

Mihm, T., McIsaac, A., Shepherd, J. J. (2019) *J Chem Phys*, **150**, 191101

Our results show that coupled cluster converges to the TDL at a rate of $N^{-1/3}$ rather than the accepted N^{-1}



Exact values were calculated using the Gell-Mann and Brueckner method:

M. Gell-Mann and K. A. Brueckner, *Phys. Rev*.**106**, 364(1957).

Conclusions:

1. **Our analysis of the CCD correlation FSE convergence rate show an $N^{-1/3}$ convergence to the TDL**
2. **We believe this will eventually cross back over to N^{-1}**
3. **Results indicated that the power law is significant enough to be worth further investigation**

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UI3 Iowa Informatics Initiative

Paper currently under review