

Abstract Submitted  
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**Using Gaussian Process Regression to Integrate the Transition Structure Factor Curve for the Many-Body Correlation Energy**<sup>1</sup> LAURA WEILER, TINA MIHM, JAMES SHEPHERD, Department of Chemistry, The University of Iowa — We apply Gaussian process regression to transition structure factor curves for a range of electron numbers and integrate to attain the correlation energy. We find that with this procedure we are able to approximate the thermodynamic limit correlation energy for the cost of relatively small system sizes. This has possible applications to the electronic structure and materials design communities as it provides a cost-effective route to the thermodynamic limit correlation energy using coupled cluster doubles calculations on the uniform electron gas.

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