

Title of doctoral thesis: **Advancement of the pair coupled cluster doubles-based molecular property calculations with quantum embedding**

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Abstract of the doctoral thesis

The works included in this thesis aim to extend the applications of pair-coupled cluster doubles (pCCD) theory. pCCD produces reliable results for strongly correlated chemical systems and performs better than other traditional quantum chemical methods. Still, achieving greater accuracy requires post-pCCD corrections, which steeply increase computational cost, limiting its widespread application. Quantum embedding approaches, which reserve accurate but high-cost methods for the active site of chemical change and approximated methods for other regions of a chemical system, can be used to circumvent this problem. In this context, two new pCCD-based embedding formulations have been implemented and tested. Both the pCCD-in-DFT and pCCD-in-pCCD methods produce reliable results across a wide range of intermolecular interactions. In particular, the latter method shows significantly better performance, as it does not depend on approximated density functionals. Additionally, estimation of molecular properties is also pertinent for practical applications with pCCD. As the traditional response-theory-based formulation for pCCD analyzed here did not meet the required level of accuracy, an alternate approach based on the expectation-value method was implemented for pCCD and post-pCCD methods. This approach produces excellent agreement with the references, at a much lower computational cost, as we bypass the need to solve the response equations. Thus, the pCCD-in-pCCD embedding method and the expectation-value-pCCD approach provide routes for large-scale simulations of challenging, complex systems.