Review of Khanh Ngoc Pham's doctoral thesis by supervisor

The thesis "Development of methods for an accurate description of cohesive properties of molecular solids" discusses reliability of various theoretical methods for the calculation of cohesive properties of molecular solids. Specifically, Khanh worked mainly on understanding methods based on random phase approximation (RPA) which were previously shown to give very promising results for binding energies of molecular solids. The goal was to understand what are the causes of errors and if they can be reduced. The work was motivated by a large interest in theoretical prediction of cohesive properties of molecular solids and the possibility to use RPA-based scheme to provide values close to reference data.

The thesis is based on two papers published in J. Chem. Phys. and another one which is in a late stage of preparation. The first one presents what could be called a manual for obtaining highly reliable many-body contributions to binding energies of molecular solids. This part is very important as the reference quality calculations are computationally expensive and it's crucial to identify settings which make the calculations tractable yet still lead to reliable results. Moreover, the accuracy of different RPA methods is discussed, including the unfortunate fact that the aforementioned promising results of standard RPA are due to substantial error cancellations. In the second paper Khanh used the reference data from the first paper and analysed the accuracy of methods that go beyond standard RPA. This is a topic that he selected out of his own interest, based on the outcomes of the first paper, and worked on it essentially independently. The final paper, which we hope to send soon for reviews, discusses the prospects of obtaining reference binding energies with the use of RPA. Note that the results of these three works were put into a logical order in the thesis so that the chapters don't correspond to papers but rather to common topics discussed in the papers.

Within his studies Khanh utilised a broad range of theoretical methods, both from solid state physics as well as from quantum chemistry, most of which had been quite new to him at the start of his studies. He's been very motivated to learn the methods and the necessary set-up and became proficient in their use so that he's now more than able to perform the work independently. He also contributed to the development of computer library that we use to set-up and analyse the calculations. Based on the results he recently identified systems which will allow to expand the understanding and is, without a need for any help, able to obtain the results. I think this illustrates that he's became a person able to identify holes in knowledge and perform the necessary work to fill them.

Let me note that Khanh presented the results on several international conferences. One notable event was a conference "Intermolecular Interactions and Properties of Gases, Liquids and Solids" in Graz in 2023 which focused on intermolecular interactions and where the results gained considerable interest of the community.

Overall, Khanh has mastered a range of theoretical methods, used them to obtain results that significantly broaden our understanding of their application for materials' simulations, and showed that he's able to perform independent scientific work. I recommend the dissertation to be accepted as a PhD thesis.

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