

Report on Narendra P. Arasu's PhD thesis "Electronic, mechanical and transport properties of molecular junctions"

In my opinion as supervisor, Mr. Narendra P. Arasu did a very good job for his PhD. He worked on the calculation of the electronic structure and conducting properties of molecular junctions using atomistic methods based on density-functional theory. He performed calculations on a series of molecular interfaces and carried out their interpretation. He also contributed to the preparation of manuscripts. As of now, his work has led to five publications in international journals.

Mr. Arasu studied the geometric properties of single molecules adsorbed on metallic substrates and the changes in electronic structure of mechanical compression of adsorbed molecules by a scanning probe tip. He also investigated the implications on conductance of aromaticity and antiaromaticity of conjugated molecules. He mastered the theoretical tools needed for this and developed new tools in the form of scripts to analyze and interpret the results. He was involved in theory-only research projects as well as jointly with experimental partners. He was often the main theory author and, in two publications, the first author.

During the course of his PhD, Mr. Arasu's scientific knowledge and skills experienced a clear progression. He started by performing the necessary calculations for his thesis research project. In the final part of his PhD, he would critically analyze his results, identify potential shortcomings, and suggest the next necessary steps. Throughout his thesis, there has been a clear and significant growth as a scientist. His PhD allowed him to produce scientific works of international quality, as evidenced by his publication record.

In short, he has fulfilled the work program I expected for this PhD and his work has resulted in several international conference presentations and publications.

With best regards,

Héctor Vázquez, PhD

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