



May 27, 2022

To whom it may concern,

I am writing this letter in strong support of Manjeera Mantina's application for a teaching position. Manjeera was a PhD student in my group from Aug 2003 to May 2008.

I am the Dorothy Pate Enright Professor at the Pennsylvania State University. My research activities focus on first-principles calculations based on density functional theory (DFT) and computational modeling of materials defects and properties and their applications to materials chemistry and process design. I published over 590 articles in peer-reviewed journals and a textbook on “Computational Thermodynamics of Materials” and graduated 31 PhD students with seven as faculty members, seven in national labs, 13 in industry, and four as postdocs.

During her PhD study, Manjeera worked on DFT-based first-principles prediction of diffusion coefficients in metallic alloys. Previously, the diffusion coefficients were predicted by the combination of the DFT-based calculations for activation energy and the molecular dynamics (MD) simulations for the prefactor. The latter is not only not accurate, but more importantly also applicable to high temperatures due to the inefficient MD sampling. By carefully studying the diffusion theory, Manjeera proposed to use the DFT-based calculations to predict the prefactor using the well-established transition-state theory, which resulted in a first-author publication in the most-rigorously reviewed physics journal, Physical Review Letter. Subsequently, she extended her approaches to other crystal structures and binary alloys systems. Her method has since become the standard method in predicting diffusion coefficients in the community.

I enjoyed working with Manjeera during her PhD study. She was not afraid of the challenging task assigned to her in developing the new approach and worked diligently by reading many references and learning from experts on DFT-based calculations. Manjeera actively participated at a number of professional conferences by giving oral and poster presentations with confidence. Furthermore, Manjeera was a great team player by sharing tasks at our various group events.

Manjeera has taken a break from professional work for caring her kids. It is great to hear that after her second kid starts going to full day school, she is now ready to make professional contributions again. I learned the wonderful news from her that she has recently obtained her teacher certification through the American Board. With her dedications to excellence and enthusiastic positive attitude, I am confident that Manjeera will be an excellent teacher and thus highly recommend her for the teaching position. If any further information is needed, please let me know.

Yours sincerely,

Zi-Kui Liu

*Dorothy Pate Enright Professor of Materials Science and Engineering*