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Ph.D., Materials Science & Engineering,  
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**Research Summary:**

Research focus is on heat transfer, thermodynamics, phase change, and reaction kinetics, with relevant applications in the fields of health, electronics, space and energy. \* Expertise in material interaction at nanoscale interfaces focusing on computational techniques to characterize materials behavior. \* Primary responsibility at ANL is to perform multimillion atom molecular dynamics simulations to investigate reactions and heat transfer in aqueous solution of nanoparticles.

**Selected Recent Publications:**

- 1) Raghavan Ranganathan, Kiran Sasikumar and Pawel Keblinski, "Realizing tuneable molecular thermal devices based on photoisomerism – is it possible?", *J. Appl. Phys.* 117, 025305 (2015).
- 2) Kiran Sasikumar and Pawel Keblinski, "Molecular dynamics investigation of nanoscale cavitation dynamics", *J. Chem. Phys.* 141, 234508 (2014).
- 3) Zhi Liang, Kiran Sasikumar and Pawel Keblinski, "Thermal transport across a substrate-thin film interface: effects of film thickness and surface roughness", *Phys. Rev. Lett.* 113, 065901 (2014).
- 4) Kiran Sasikumar, Zhi Liang, David G. Cahill and Pawel Keblinski, "Curvature induced phase stability of an intensely heated liquid", *J. Chem. Phys.* 140, 234506 (2014).
- 5) Zhi Liang, Kiran Sasikumar and Pawel Keblinski, "Liquid phase stability under an extreme temperature gradient", *Phys. Rev. Lett.* 111, 225701 (2013).
- 6) Kiran Sasikumar and Pawel Keblinski, "Effect of chain conformation in the phonon transport across a Si- polyethylene single-molecule covalent junction", *J. Appl. Phys.* 109, 114307 (2011).