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### ABSTRACT:

Through multiscale analyses we introduce harvesting of resonant optical phonons in semiconductors, with three new concepts:

- phonon recycling (absorption) in in graded heterojunction for partial reversal of the joule heating,
- phonovoltaic for direct hot-phonon energy conversion, and
- phonocatalysis with phonon-controlled chemisorbed dissociation.

In reversing the joule heating through in-situ phonon recycling (pR), we tune a heterojunction barrier height to optical phonons and optimize it for GaAs:Al electron channel for maximum phonon absorption. We calculate the pR efficiency of this partial reversal of phonon emission.

In phonovoltaic (pV) with nonequilibrium optical phonon source and phonon generation of charge pairs in p-n junction to generate power, we define the pV figure of merit and explore the optimal material for efficient room-temperature pV. We search for pV materials and tune the graphene compounds (e.g., hC:BN) bandgap to its optical phonons and evaluate the efficiency. In phonocatalysis (pC) with ab initio molecular dynamics we show the chemisorbed dissociation of XeF<sub>6</sub> on h-BN surface leads to formation of XeF<sub>4</sub> and two surface F/h-BN bonds. We show that the chemisorbed dissociation (the pathway activation ascent) requires absorption of large-energy optical phonons. Then using progressively heavier isotopes of B and N atoms, we show that limiting these high-energy optical phonons inhibits the chemisorbed dissociation, i.e., controllable pC.

### BIOGRAPHY:

Massoud Kaviany (Ph.D. UC-Berkeley 1979) is Professor in Department of Mechanical Engineering and in Applied Physics Program, University of Michigan, since 1986. His interest is in heat transfer physics. He has authored Heat Transfer Physics, 2nd Edition 2014 and Essentials of Heat Transfer 2011, by Cambridge University Press. He was Chair of ASME Committee on Theory and Fundamental Research in Heat Transfer, is Associate Editor of Nanoscale and Microscale Thermophysical Engineering, ASME Life Fellow and APS Fellow, and recipient of University of Michigan Engineering 2003 Education Excellence Award, ASME 2002 Heat Transfer Memorial Award (Science), 2010 Harry Potter Gold Medal (Thermodynamics Science), and 2013 Heat Transfer Division 75th Anniversary Medal.