工学系研究科専攻間横断型教育プログラム
「機械システム・イノベーション」

最先端融合科学イノベーション
教育研究コンソーシアム

東京大学 THE UNIVERSITY OF TOKYO

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Resonant phonon harvesting

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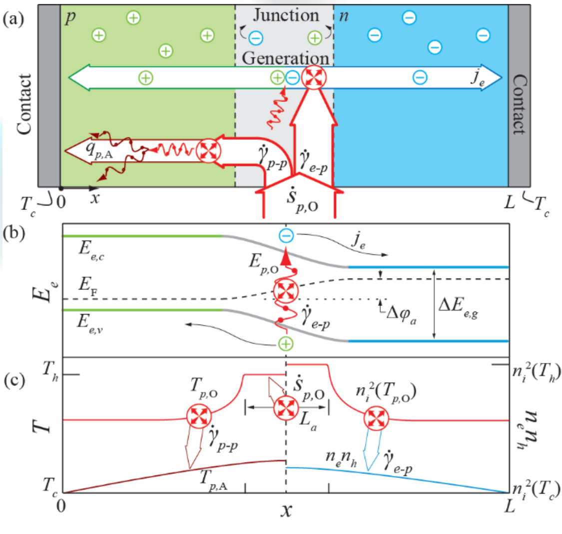
Through multiscale analyses we introduce harvesting of resonant optical phonons in semiconductors, with three new concepts:

- *phonon recycling* (absorption) in in *graded heterojuction* 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 phonocatalysics (pC) with *ab initio* molecular dynamics we show the chemisorbed dissociation of XeF_6 on h-BN surface leads to formation of XeF_4 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.



主催：　東京大学大学院工学系研究科「機械システム・イノベーション」プログラム（GMSI）
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