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Generation of hot plasmonic carriers, thermal effects and plasmonic photochemistry in metal nanocrystals ALEXANDER GOVOROV, Ohio University, HUI ZHANG, Rice University, LUCAS VÁZQUEZ, Ohio University, YURII GUN'KO, University of Dublin, Ireland, MIN OUYANG, University of Maryland — We investigate the effects of generation of hot plasmonic carriers and heat in metal and hybrid nanostructures. In our theory, the problem of hot-electron generation is calculated using the quantum-mechanical approach based on the DFT theory and the equation of motion of the density matrix [1], whereas the problem of heat release is treated classically. The energy distribution of optically-excited plasmonic carriers is very different in metal nanocrystals with large and small sizes. We found that the hot-electron generation is efficient only for nanocrystals with very small sizes or in nanocrystals with plasmonic hot spots. The physical reason for the above behaviors is non-conservation of momentum in a nanocrystal. Using the newly-developed kinetic DFT theory, we also describe the effect of breaking of the plasmon resonance into multiple peaks in small nanocrystals. Finally, the generation of plasmonic holes via the interband transitions leads to efficient photochemistry [2]. The results obtained in this study can be used to design a variety of plasmonic nanodevices for photocatalysis and photodetectors.

[1] A.O. Govorov, et al., *NanoToday*, 9, 85 (2014).
[2] L. Weng, et al., *Nature Commun.* 5, 4792 (2014).

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