University of Delaware MRSEC Theoretical and computational modeling of spintronic THz emitters

A. Kefayati, J. Varela-Manjarres, M. B. Jungfleisch, J. Q. Xiao, and B. K. Nikolić **Department of Physics and Astronomy**

Key Advances

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- Ultrafast-light-driven magnetic heterostructures exhibit concurrent demagnetization and emission of THz radiation.
- Despite being a primary experimental probe of spin-charge coupled dynamics and transport, there have been virtually no calculations of THz radiation from such systems since the inception of this field in 1996.
- We solved this longstanding problem by introducing two new complementary frameworks, which combine time-dependent density functional theory (TDDFT) or time-dependent nonequilibrium Green's functions (TDNEGF) with Jefimenko solutions of the Maxwell equations.
- Our solutions make it possible to predict (and doubly confirm) a new effect (charge current pumping by ultrafast demagnetization), while concurrently explaining the microscopic origin of conjectured interlayer spin current.

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Fig. Illustration of ferromagnet/normal-metal (FM/NM) heterostructure whose FM laver is driven by femtosecond laser pulse (fsLP) and where our **TDDFT+Jefimenko TDNEGF+Jefimenko** theoretical/computational or approaches predict pumping of intralayer charge current I^x_{EM} and interlayer spin current I^z_{Sa} by demagnetization dynamics. Both eventually contribute to emitted THz radiation, which we compute for the first time from first principles theory.



