

First-Principles QuantumATK Calculations

of Microscopic Physical Parameters for Optical Switchable Magnetic Materials

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QuantumATK

QuantumATK is an integrated software suite for atomic-scale modelling. It combines the power of a scripting engine, based on Python scripting, with the ease-of-use provided by an intuitive graphical user interface.

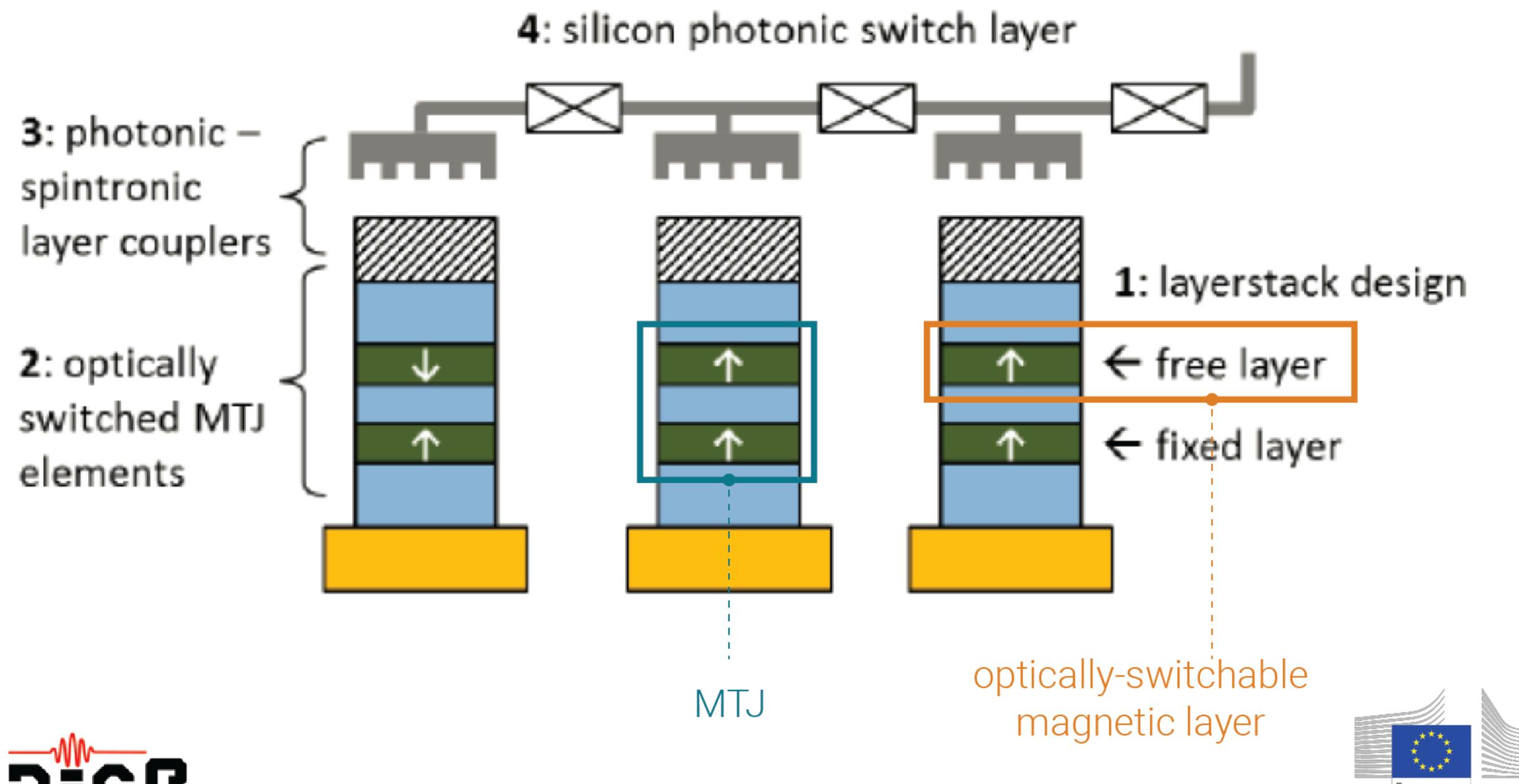


www.quantumwise.com

Simulation Engines
DFT-PlaneWave → 10^2 - 10^3 atoms
DFT-LCAO → 10^3 - 10^4 atoms
Semi-Empirical 10^5 atoms
ForceField → 10^5 - 10^7 atoms
NEGF device simulations

Objectives

The simulation tools developed by Synopsys QuantumATK have been applied for atomistic study of magnetic materials and individual components comprising optically switchable RAM. Synopsys QuantumATK focuses on the component level atomic-scale simulations.



Theory

Spin dynamics via parametric coupling of Density Functional Theory (DFT) to the Landau-Lifshits-Gilbert (LLG) model.

More Details on LLG Model: Sanvitto et al., arXiv:1710.00574v1

$$\frac{\partial \mathbf{S}_i}{\partial t} = -\gamma \mathbf{S}_i \times \mathbf{H}_i + \lambda \mathbf{S}_i \times \frac{\partial \mathbf{S}_i}{\partial t} + \frac{1}{\mu_i} \mathbf{T}_i(V, \{\mathbf{S}_i\})$$

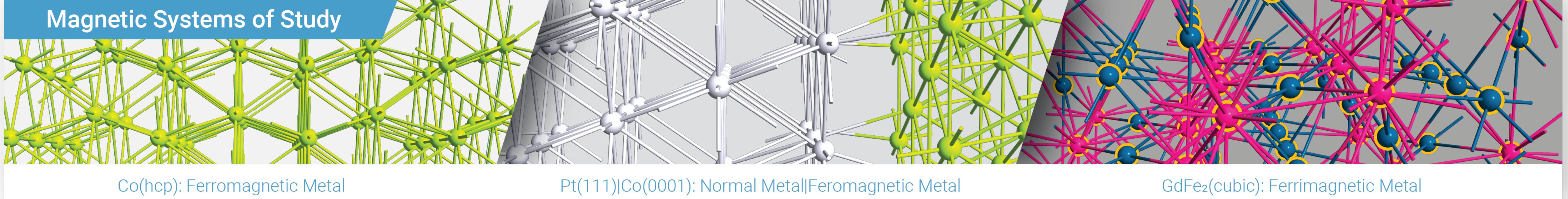
■ Parameters computed using DFT-LCAO or Plane Wave pseudopotential method in QuantumATK (magnetization, exchange coupling constants, STT)
 ■ Parameters taken from the experiment (Gilbert damping, λ)

$$\mathbf{H}_i(t) = -\frac{1}{\mu_i} \frac{\partial \mathcal{H}}{\partial \mathbf{S}_i} + \xi_i(t), \quad \mathbf{T}_i: \text{Spin Transfer Torque (STT)}$$

$\xi_i \propto \lambda k_B T / \gamma$ **Stochastic field:** It takes into account a finite temperature effect on magnetization

$$\mathcal{H} = -\sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j \quad \text{Heisenberg model with exchange coupling constants } J_{ij}$$

Magnetic Systems of Study



Results

Ab-Initio Derived Microscopic Parameters (QuantumATK)

Bulk Co

Magnetization [QuantumATK] = $1.64 \mu_B/\text{Co-atom}$
 Magnetization [Experimental] = $1.72 \mu_B/\text{Co-atom}$

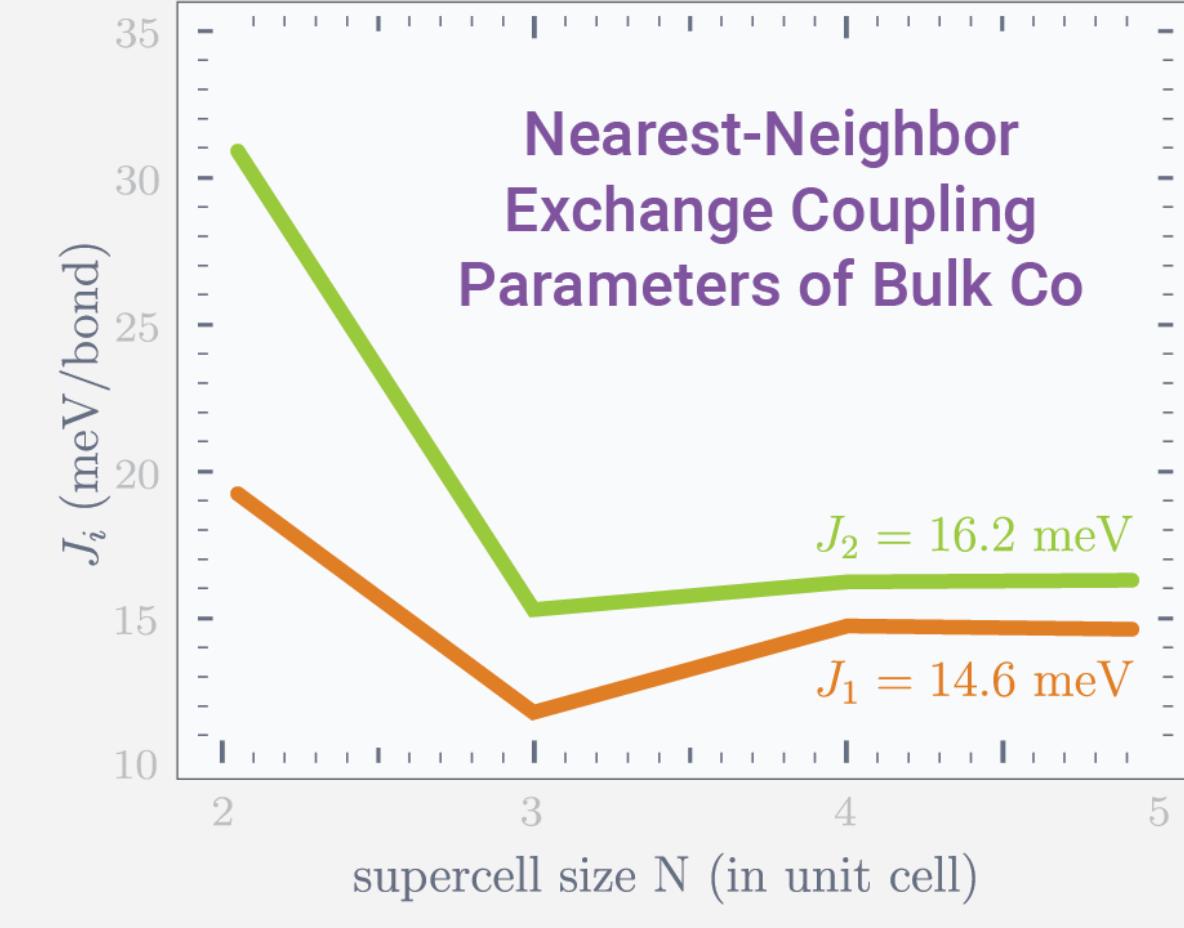
Pt(111)|Co(0001) Heterostructure

Monolayer (#)	Pt (1)	Pt (2)	Pt (3)	Pt (4)	Co (1)	Co(2)
Magnetization (μ_B/atom)	0.23	0.12	0.12	0.23	1.91	1.91
Magnetization in Bulk (μ_B/atom)	0.00	0.00	0.00	0.00	1.64	1.64

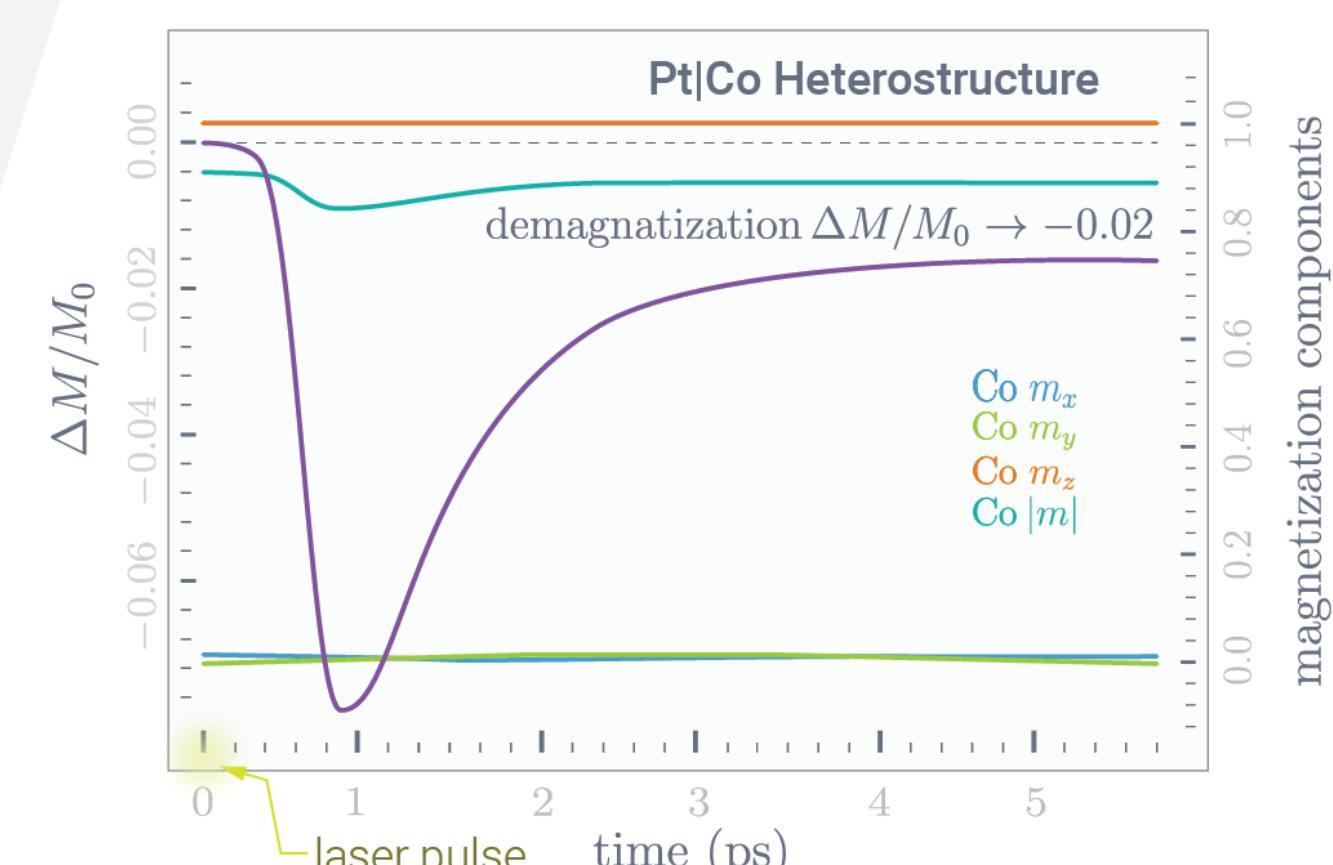
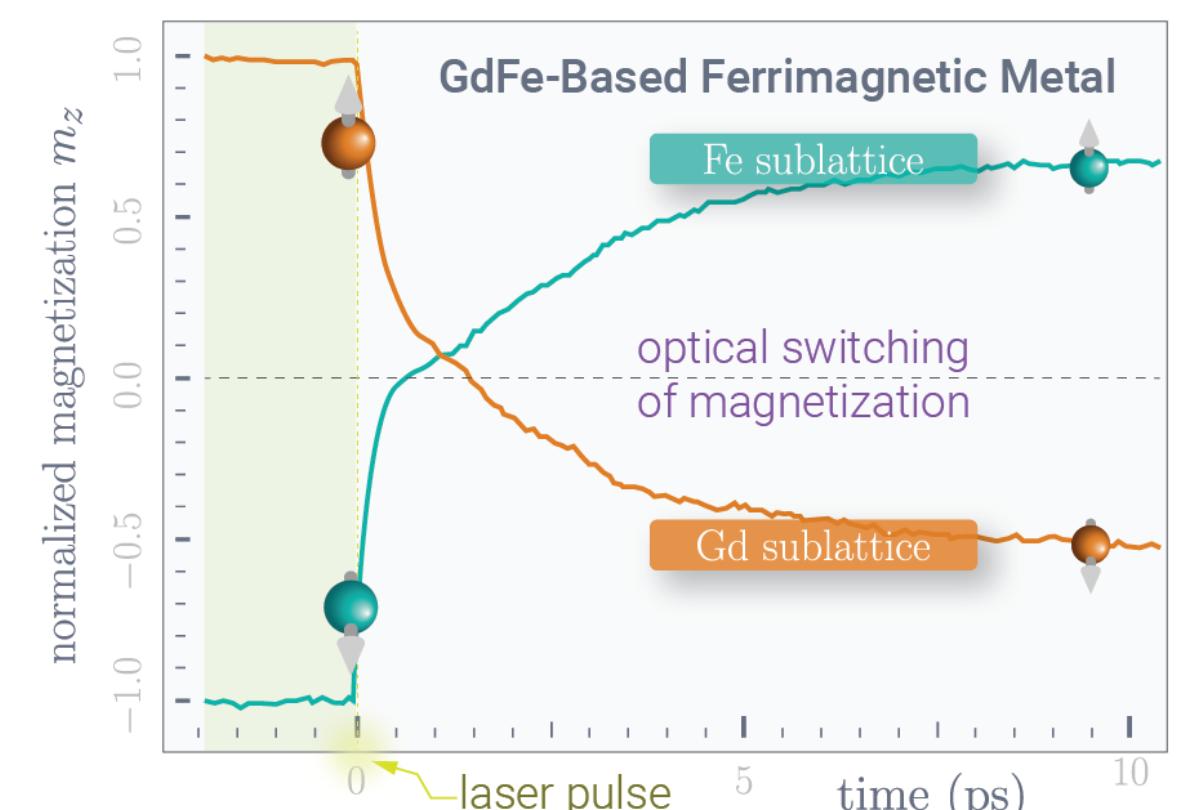
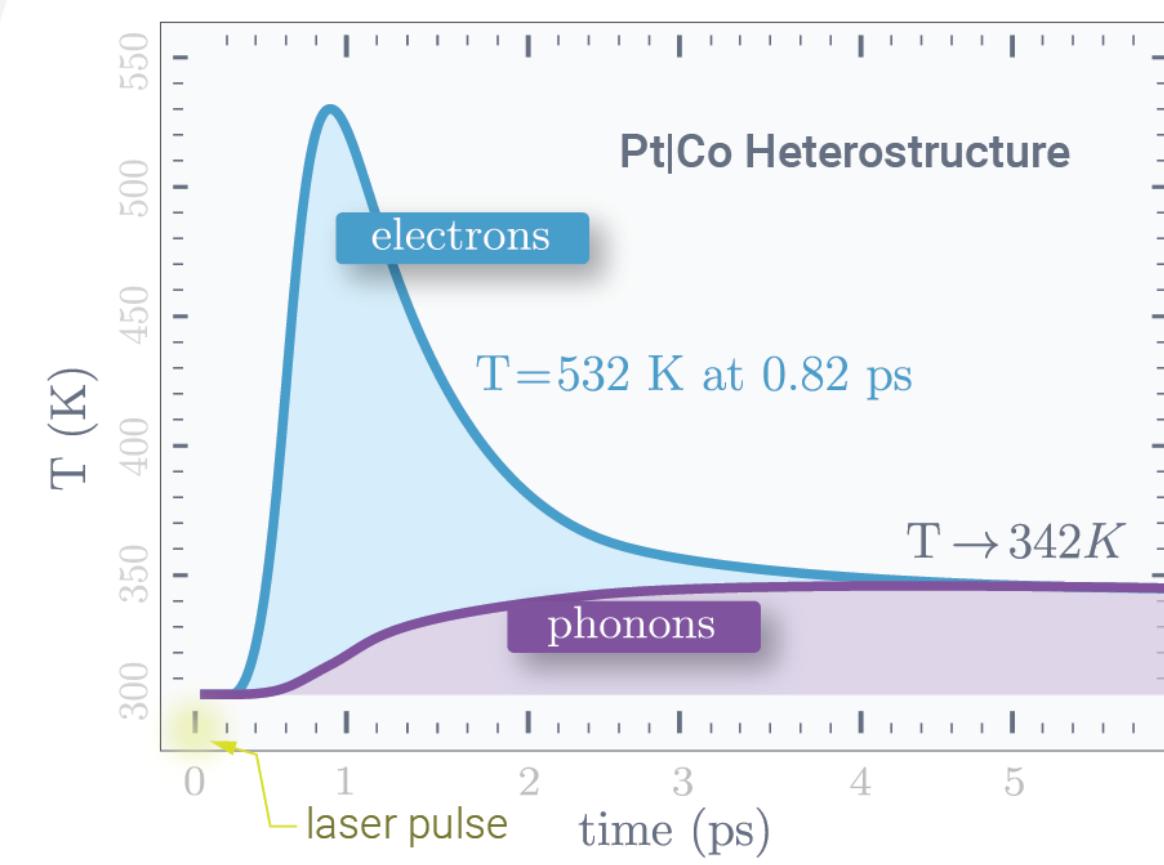
Nearest-Neighbor Exchange Coupling Parameters of Pt|Co:

$J_1 = 35.4 \text{ meV}$ for (2.392\AA) Co-Co bond
 $J_1 = 11.6 \text{ meV}$ for (2.800\AA) Co-Co bond
 $J_1 = 2.0 \text{ meV}$ for (2.646\AA) Co-Pt bond

- Ab initio calculated magnetization of bulk Co agrees with experiment.
- Accurate calculation of J-parameters of Co requires large supercells.
- Pt layer becomes slightly magnetic due to proximity effect at the Pt|Co interface.
- Strain at the Pt|Co interface strongly affects coupling constants, compared to bulk Co.



Magnetization Dynamics



- Upon illumination, the electron temperature of the magnetic system increases rapidly from $T=300$ to 532 K .
- Subsequently, the electron subsystem transfers the excess energy to the phonon subsystem, increasing the phonon temperature.
- The two subsystems equilibrate at the temperature of $T=342 \text{ K}$, and the magnetic system reaches its new equilibrium state.
- Upon illumination, total magnetization of the magnetic system drops by about 8%, when the electron temperature reaches its maximum at $T=532 \text{ K}$.
- Magnetization partially recovers when the magnetic system reaches its new equilibrium state at $T=342 \text{ K}$, decreasing by 2% from its initial value, M_0 .

VAMPIRE Software Package (<http://vampire.york.ac.uk/>),
 Evans et al., J. Phys.: Cond. Matt. 26, 103202 (2014)

Conclusions

- QuantumATK was used to calculate the magnetic properties of spintronics materials: saturation magnetization and Heisenberg exchange coupling parameters.
- Ab-initio calculated microscopic physical parameters were then adopted as input for the empirical LLG model to study spin dynamics in magnetic systems.
- Demagnetization of the Pt|Co heterostructure and optical switching of magnetization in a GdFe-based system were demonstrated using the VAMPIRE code.