Stability and lifetimes of magnetically coupled Fe nanostructures on Pt(111)

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Abstract

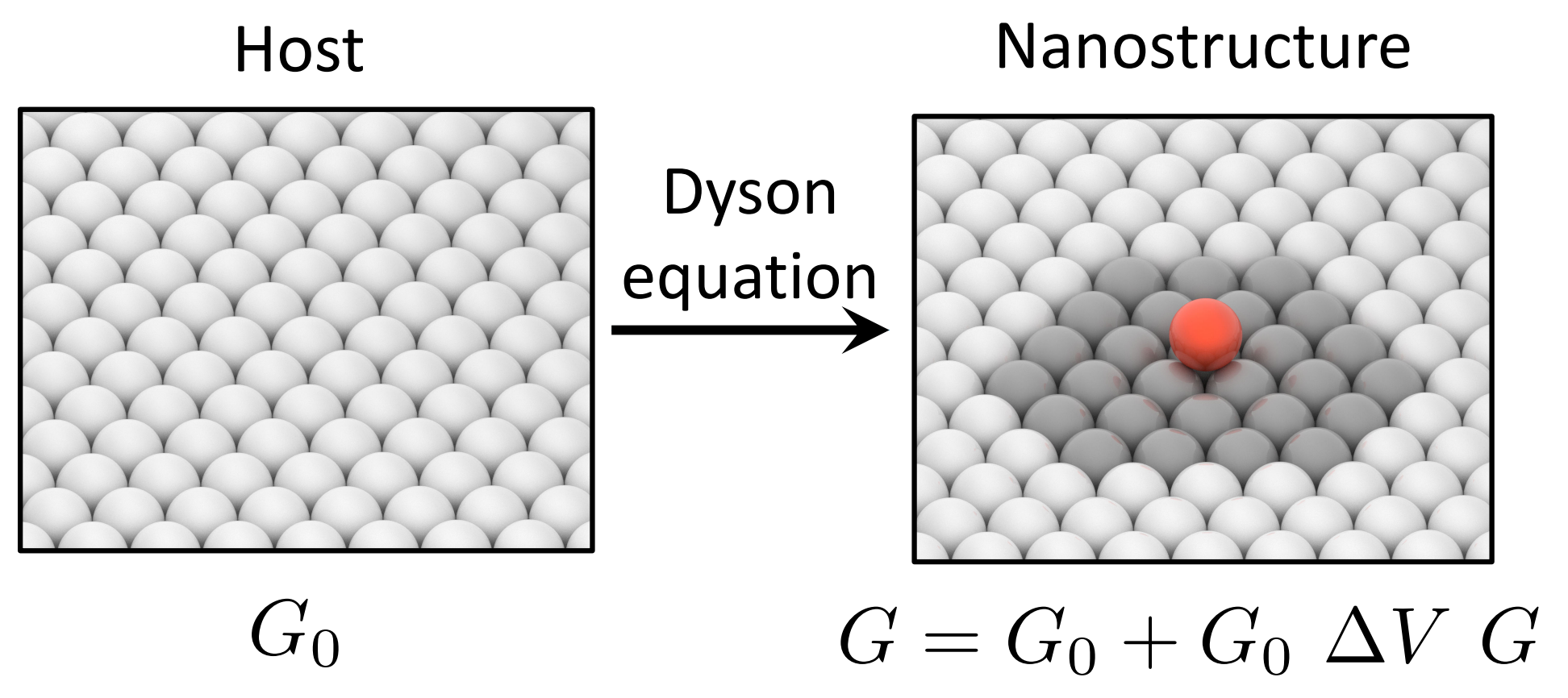
Nanostructures made of a few magnetic atoms are of great interest not only for studying the physics of magnetism at the atomic scale but also for possible use as magnetic bits or logic elements. Ho adatoms are found to be stable on the MgO/Ag(001) surface [1], while Fe trimers are stable on the metallic Pt(111) surface [2]. The properties of Fe trimers (and adatoms) on Pt(111) were found to depend strongly on how they are stacked on the surface [2,3]. To understand and manipulating their magnetic stability, knowledge of the interactions with the surroundings, in particular other magnetic entities, is of paramount importance.

The magnetic interactions between Fe atoms on Pt(111) have been experimentally mapped and also extracted from first-principles calculations [4]. They comprise not only the isotropic Heisenberg exchange interactions but also chiral Dzyaloshinskii-Moriya interactions. In this contribution, we present our results for the magnetic interactions between several types of Fe nanostructures: adatom-dimer, adatom-dimer, adatom-trimer, and trimer-trimer. The influence of the stacking site is explored, as well as a so-far overlooked type of magnetic interaction, the symmetric exchange. The dependence of the interactions not only on the distance but also on the relative arrangement of the nanostructures has a strong influence on the magnetic stability and the corresponding lifetimes of the magnetic states. This is borne out quantitatively via a newly developed scheme that combines data from first-principles calculations with a master equation based on an Anderson-Appelbaum-type model.

[1] F. Donati *et al.*, Science **352**, 318 (2016)
[2] J. Hermenau *et al.*, Nat. Commun. **8**, 642 (2017)
[3] A. A. Khajetoorians *et al.*, PRL **111**, 157204 (2013)
[4] A. A. Khajetoorians *et al.*, Nat. Commun. **7**, 10620 (2016)

DFT and exchange interactions

- Electronic and magnetic structure calculations using **density functional theory** (DFT)
- **Korringa-Kohn-Rostoker** (KKR) Green function method – real space approach
- Embedding nanostructures on surfaces



G_0

$$G = G_0 + G_0\,\Delta V\,G$$

- Extract exchange interactions and magnetic anisotropies utilizing the magnetic force theorem [5,6] yielding a **classical** Heisenberg Hamiltonian

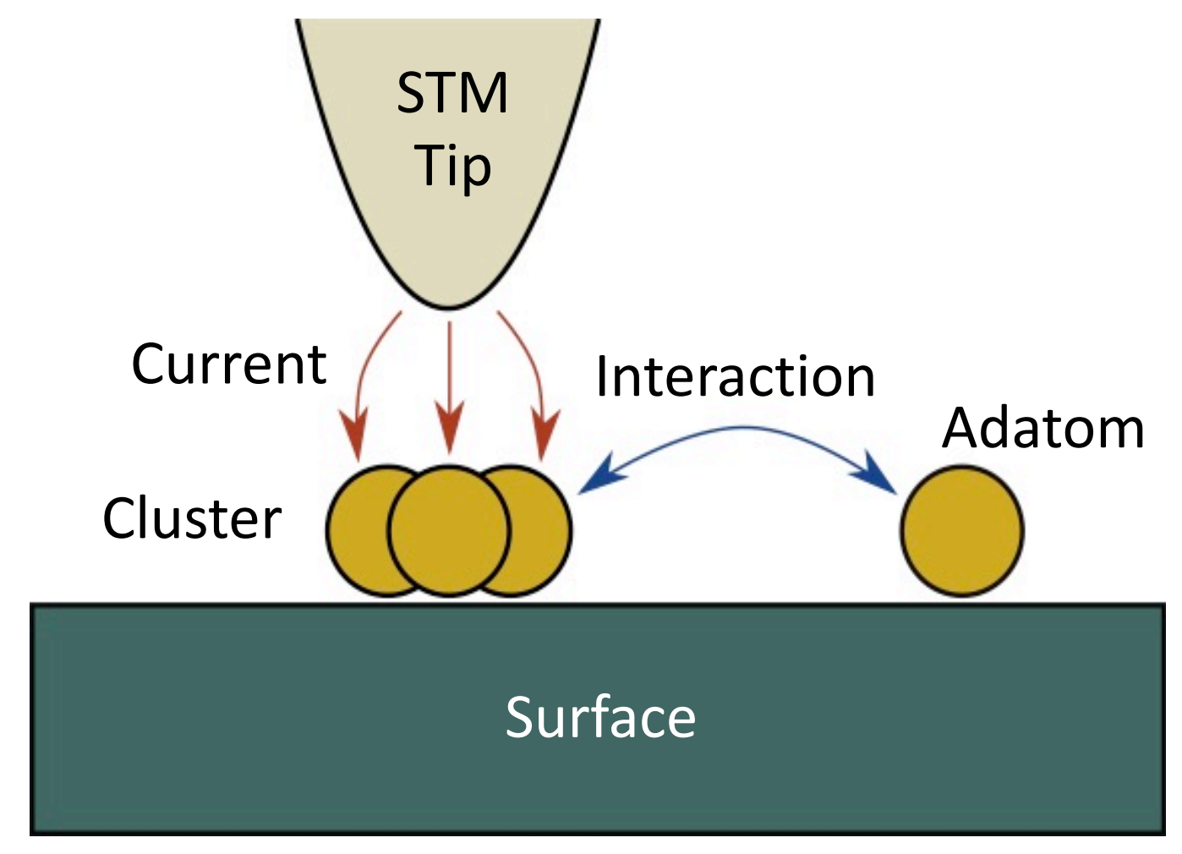
$$\mathcal{H} = \mathcal{H}_{\mathrm{MAE}}\left(\{\hat{e}_i\}\right) + \frac{1}{2}\sum_{ij}\hat{e}_i J_{ij}\hat{e}_j - \vec{B}\cdot\sum_i \vec{m}_i$$

with the 3×3 matrix of pair interactions $\hat{e}_i = \dfrac{\vec{m}_i}{|\vec{m}_i|}$

$$J = J^{\mathrm{iso}} + J^{\mathrm{sym}} + J^{\mathrm{anti\text{-}sym}}$$

[5] D. S. G. Bauer, Ph.D. thesis, RWTH Aachen (2014)
[6] A. I. Liechtenstein et al., JMMM **67**, 65-74 (1987)

Telegraph noise model



- **Quantum** Heisenberg model describing magnetic atoms
- Applebaum Hamiltonian describes the interactions of the magnetic cluster with the surface and the tip [7]

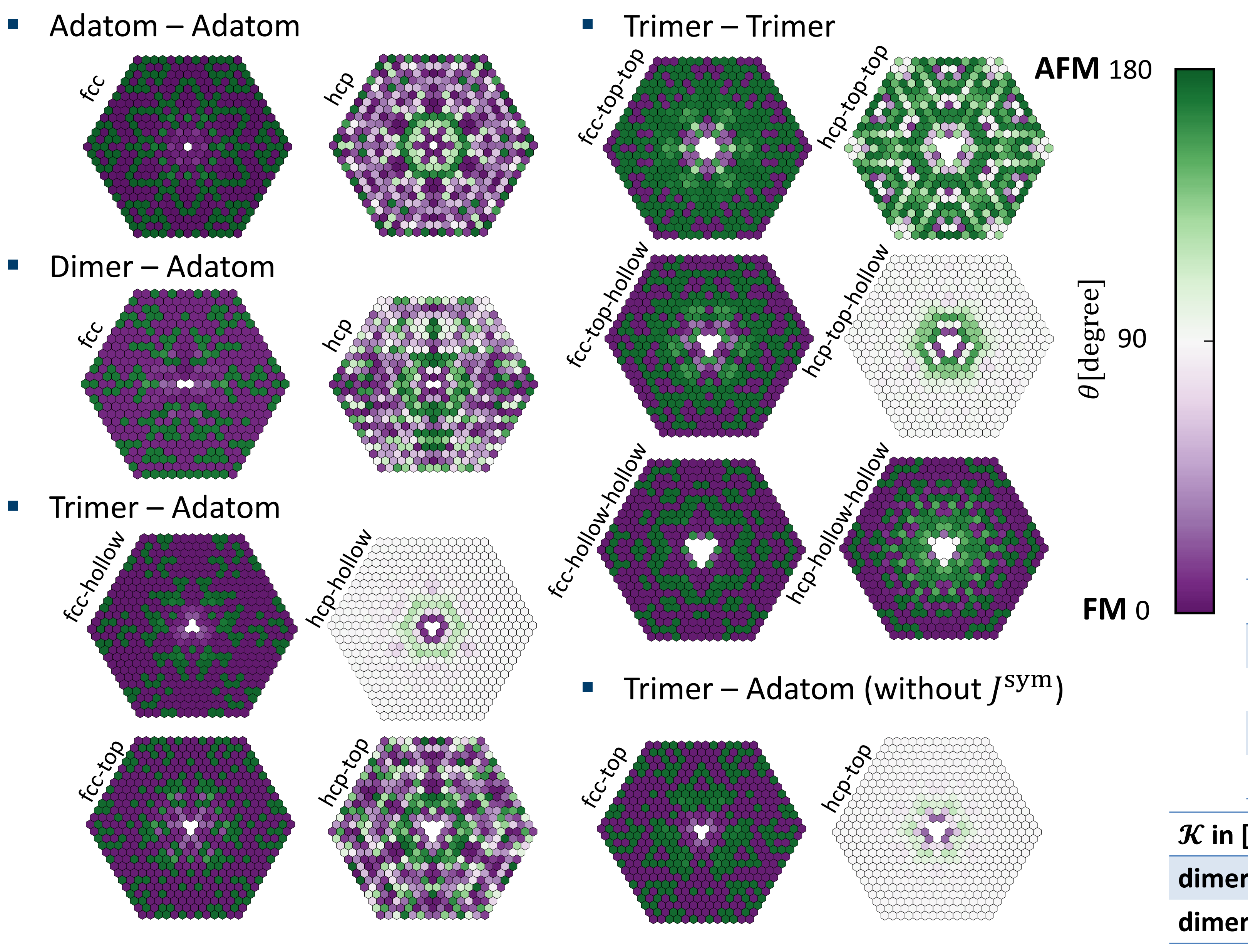
$$\mathcal{V} = \sum_{\alpha,\eta,\eta',i} T_i^{\eta,\eta',\alpha} S_i^{\alpha} c_\eta^\dagger \frac{\sigma^\alpha}{2} c_{\eta'}$$

- Lifetimes from a master equation approach combined with Fermi's Golden rule [7]

$$\frac{\mathrm{d}P_M}{\mathrm{d}t} = \sum_{M'} P_{M'} W_{M'M} - P_M \sum_{M'} W_{MM'}$$

[7] Delgado *et al.* PRB **82**, 134414 (2010)

Ground-state spin configuration


- Adatom – Adatom
- Dimer – Adatom
- Trimer – Adatom
- Trimer – Trimer
- Trimer – Adatom (without J^{sym})

- Minimize generalized Heisenberg model
- θ is the averaged angle between the spins of the two clusters in their ground states
- MAE obtained from DFT and from the Heisenberg model (macro-spin)

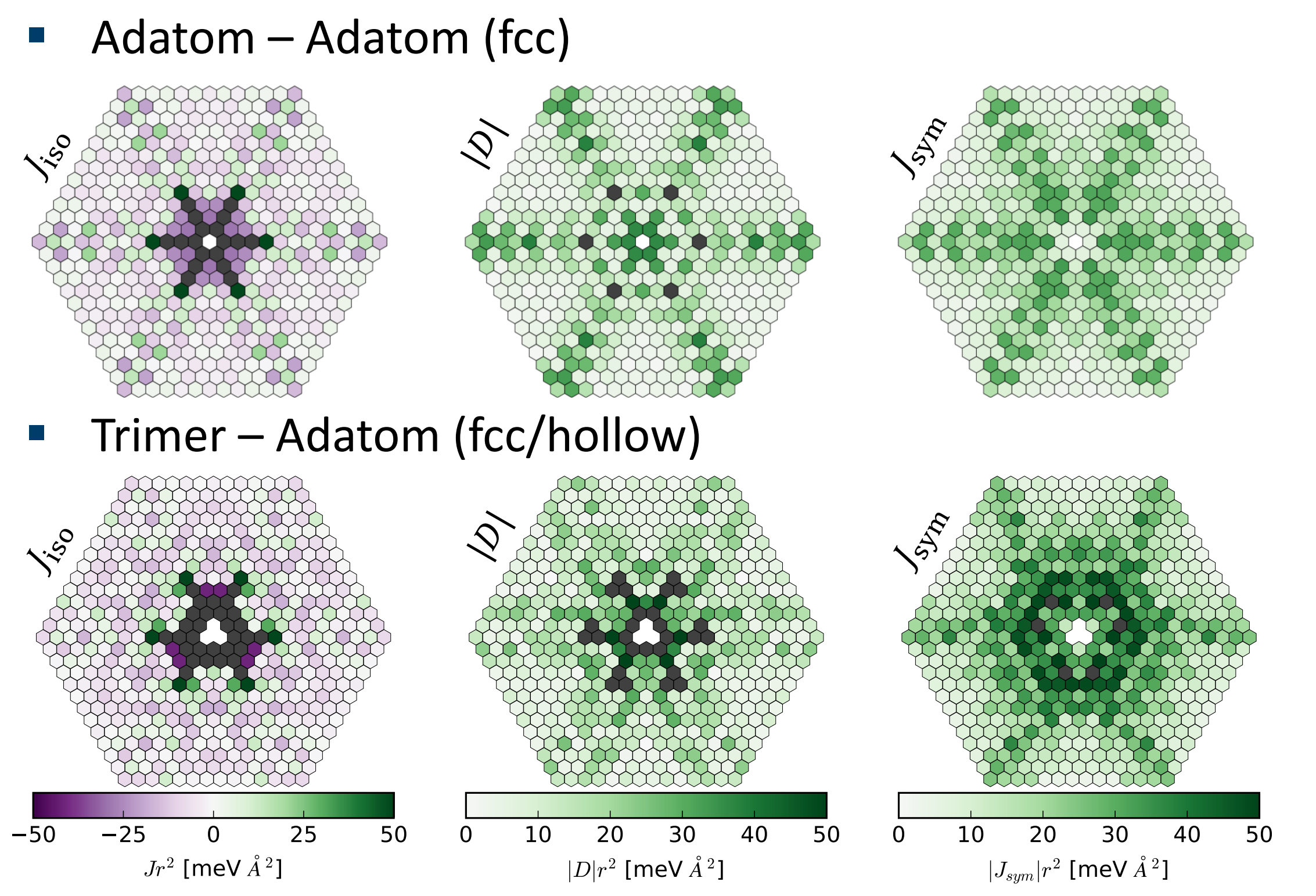
$$\mathcal{H}_{\mathrm{MAE}} = \sum_i \hat{e}_i \mathcal{K}^i \hat{e}_i$$

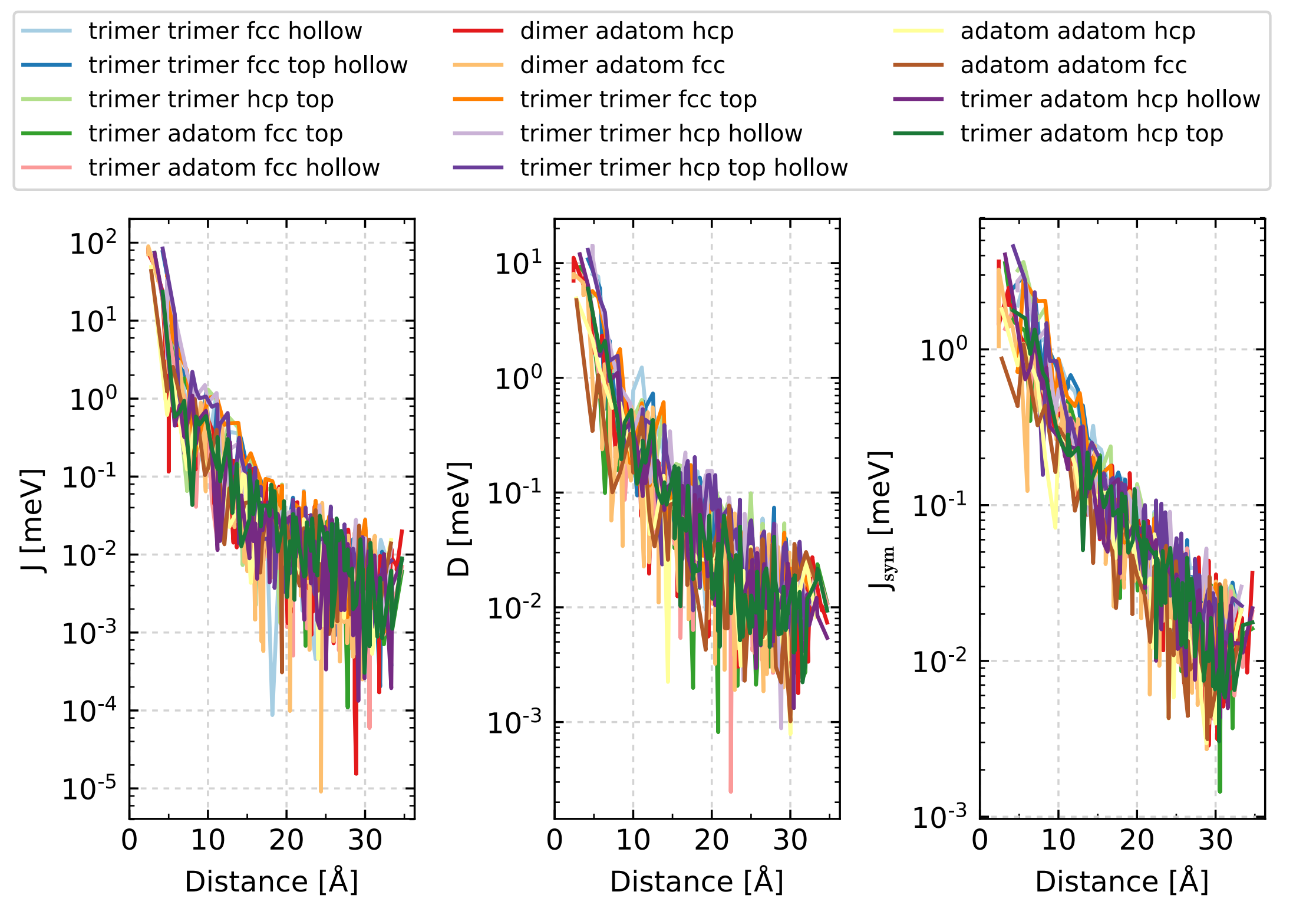
$$\mathcal{K} = \begin{pmatrix} \mathcal{K}_{xx} & \mathcal{K}_{xy} & \mathcal{K}_{xz} \\ \mathcal{K}_{xy} & \mathcal{K}_{yy} & \mathcal{K}_{yz} \\ \mathcal{K}_{xz} & \mathcal{K}_{yz} & \mathcal{K}_{zz} \end{pmatrix}$$

$\mathcal{K}$ in [meV]	$\mathcal{K}_{zz}^{\mathrm{on-site}}$		$\mathcal{K}_{zz}^{\mathrm{macro}}$	
	fcc	hcp	fcc	hcp
adatom	-1.92	0.68	-1.92	0.68
trimer-hollow	-0.88	-0.80	-7.00	-0.62
trimer-top	-0.61	-0.84	-0.67	1.27

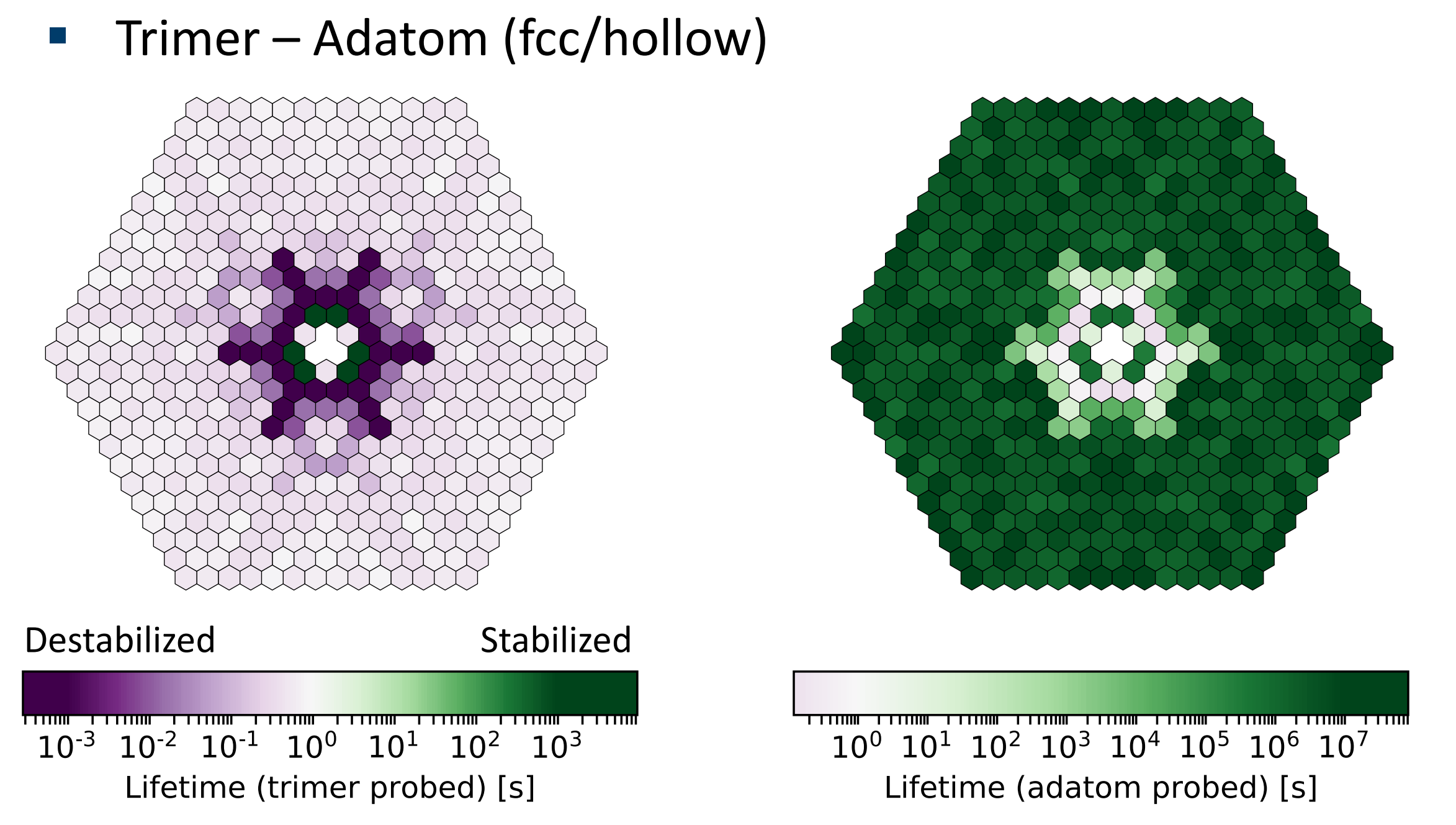
$\mathcal{K}$ in [meV]	$\mathcal{K}_{xx}$	$\mathcal{K}_{yy}$	$\mathcal{K}_{yz}$	$\mathcal{K}_{xx}^{\mathrm{macro}}$	$\mathcal{K}_{yy}^{\mathrm{macro}}$	$\mathcal{K}_{yz}^{\mathrm{macro}}$
dimer fcc	0.02	1.63	-0.34	0.73	4.33	-0.67
dimer hcp	-0.73	0.06	0.06	-2.68	0.15	0.82

Magnetic exchange interactions


- Adatom – Adatom (fcc)
- Trimer – Adatom (fcc/hollow)

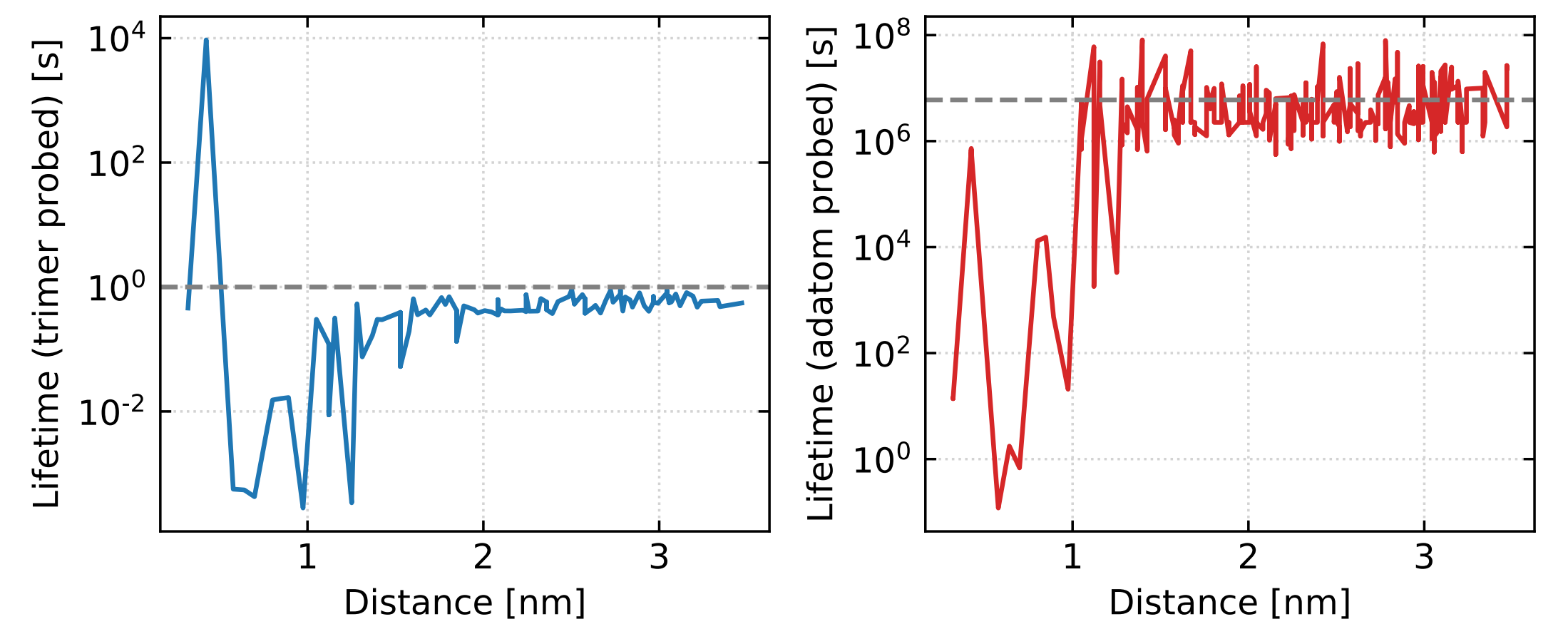


Telegraph noise lifetimes


- Trimer – Adatom (fcc/hollow)

Probed isolated trimer lifetime 1 s
Probed isolated adatom lifetime $\sim 7\times10^{-6}$ s

Unprobed isolated trimer lifetime $\sim 6\times10^{6}$ s
Unprobed isolated adatom lifetime ~ 0.045 s



- Model parameter: Ratio between the coupling to the tip and to the surface $\frac{\nu_{\mathrm{tip}}}{\nu_{\mathrm{surface}}} = 0.070$, as obtained in Ref. [2] at a voltage of 5 V. Unknown prefactor fixed such that the isolated trimer has a lifetime of 1 s.

Macro spin approximation

- Cluster with >1 atoms contains exchange interactions [2]

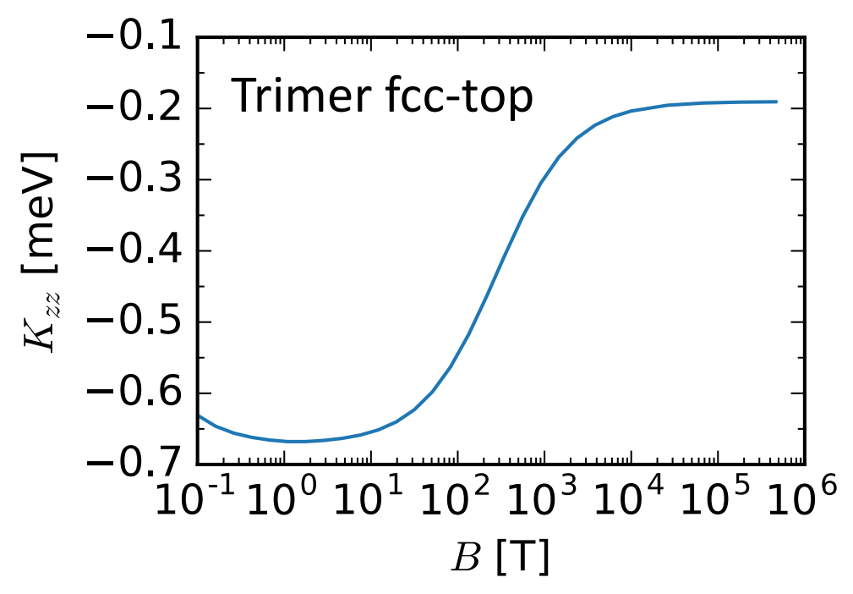
$$\mathcal{H}^{\mathrm{clust}} = \mathcal{H}_{\mathrm{MAE}}^{\mathrm{clust}}\left(\{\hat{e}_i\}\right) + \frac{1}{2}\sum_{ij}\hat{e}_i J_{ij}\hat{e}_j - \vec{B}\cdot\sum_i \vec{m}_i$$

- The macro spin absorbs the internal interactions in the MAE

$$\mathcal{H}^{\mathrm{macro}} = \mathcal{H}_{\mathrm{MAE}}^{\mathrm{macro}}(\vec{M}) - \vec{B}\cdot\vec{M}$$

- Mapping total energies of the cluster including an external magnetic field to the macro spin model

$$\begin{aligned} & E^{\mathrm{clust}}[\{\theta_i(\vec{B}),\phi_i(\vec{B})\}] \\ \Rightarrow\quad & E^{\mathrm{macro}}[\theta(\vec{B}),\phi(\vec{B})] \\ \Rightarrow\quad & \mathcal{H}_{\mathrm{MAE}}^{\mathrm{macro}} \end{aligned}$$



Conclusions

The magnetic structures of composite nanostructures are determined by the magnetic anisotropy of the constituents and by their RKKY-coupling. We showed using the example of a fcc-hollow trimer coupled to an adatom that the probed trimer is significantly destabilized for intermediate distances between the trimer and the adatom. In particular, we found a correlation between the DMI strength and the destabilization of the trimer. In the long distance regime, the probed adatom shows the signature of the unprobed trimer by inducing an asymmetry in its own fast (experimentally not measurable) switching rate.

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