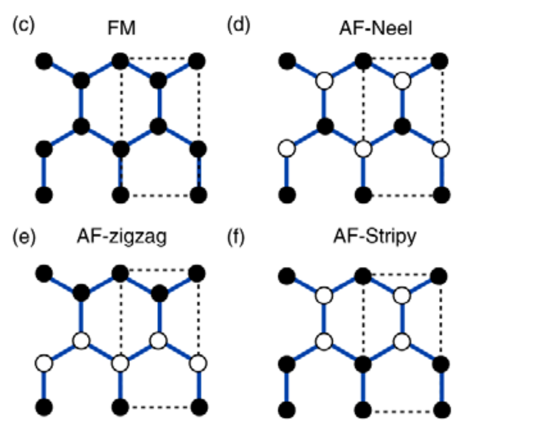
Full Hamiltonian

$$\mathbf{H} = -2\mathrm{J}_1 \sum_{\langle i,j\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - 2\mathrm{J}_2 \sum_{\langle\langle i,j\rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - 2\mathrm{J}_3 \sum_{\langle\langle\langle i,j\rangle\rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \mathrm{D} \sum_{i} |S_i^z|^2 - 2\lambda \sum_{\langle i,j\rangle} S_i^z S_j^z$$

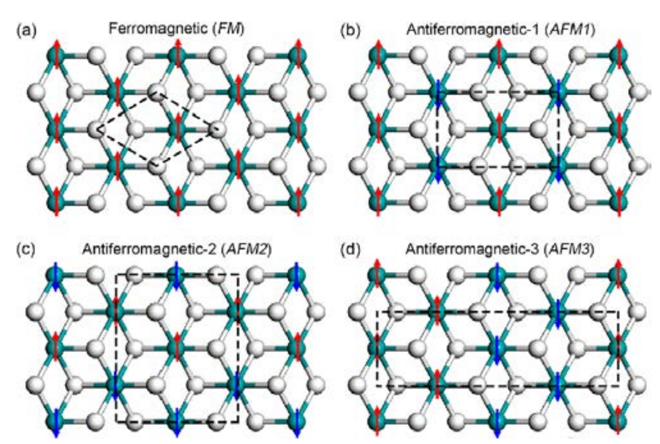
$\langle i,j\rangle$, $\langle\langle i,j\rangle\rangle$, and$\langle\langle\langle i,j\rangle\rangle\rangle$ denotes the nearest, second, and third neighbor spins.
$\mathrm{J}_{1,2,3}$ are the Heisenberg exchange constants between nearest, second, and third neighbor spins.

For Cubic lattice: $\mathrm{N}_1 = \mathrm{N}_2 = \mathrm{N}_3 = 4$
For Hexagonal/Honeycomb lattice: $\mathrm{N}_1 = 3, \mathrm{N}_2 = 6, \mathrm{N}_3 = 3$
For Triangular lattice: $\mathrm{N}_1 = \mathrm{N}_2 = \mathrm{N}_3 = 6$
##

Heisenberg Exchange Constant

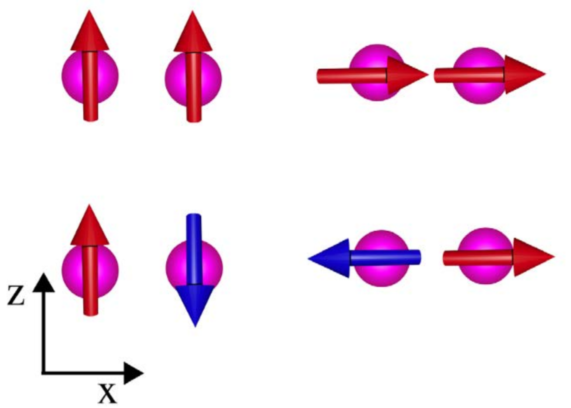


Hexagonal example [1]
$\mathrm{E}_{FM/Neel} = -E_0 - (\pm 3J_1 + 6J_2 \pm 3J_3)\lvert\vec{S}\rvert^2 - D\lvert\vec{S_z}\rvert^2$
$\mathrm{E}_{Zigzag/Stripy} = -E_0 - (\pm J_1 - 2J_2 \mp 3J_3)\lvert\vec{S}\rvert^2 - D\lvert\vec{S_z}\rvert^2$



Triangular example[2]
$\mathrm{E}_{FM} = -E_0 - (6J_1 + 6J_2)\lvert\vec{S}\rvert^2 - D\lvert\vec{S_z}\rvert^2$
$\mathrm{E}_{AFM1} = -E_0 - (-2J_1 - 2J_2)\lvert\vec{S}\rvert^2 - D\lvert\vec{S_z}\rvert^2$
$\mathrm{E}_{AFM3} = -E_0 - (2J_1 - 2J_2)\lvert\vec{S}\rvert^2 - D\lvert\vec{S_z}\rvert^2$

Single Ion Anisotropy + Anisotropy Symmetric Exchange[3]

	Hexagonal example (just considering the nearest neighbors)
	$\mathrm{E}_{FM,z} = -E_0 - D\left\|\vec{S}\right\|^2 - 3(J+\lambda)\left\|\vec{S}\right\|^2$
	$\mathrm{E}_{AFM,z} = -E_0 - D\left\|\vec{S}\right\|^2 + 3(J+\lambda)\left\|\vec{S}\right\|^2$
	$\mathrm{E}_{FM,x} = -E_0 - 3J\left\|\vec{S}\right\|^2$
	$\mathrm{E}_{AFM,x} = -E_0 + 3J\left\|\vec{S}\right\|^2$

[1] N. Sivadas, M. W. Daniels, R. H. Swendsen, S. Okamoto, and D. Xiao, Phys. Rev. B **91**, 235425 (2015).

[2] Q. Wu, Y. Zhang, Q. Zhou, J. Wang, and X. C. Zeng, J. Phys. Chem. Lett. **9**, 4260 (2018).

[3] J. L. Lado, Fernández-Rossier, Joaquín, 2D Materials **4**, 035002 (2017).