

IFMP Seminar

Date Tuesday, January 10, 2023, at 14:50

REC/C213

BigBlueButton:

<https://selfservice.zih.tu-dresden.de/link.php?m=188428&p=bb22c122> (TUD)

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Speaker **Stanislav Avdoshenko**

IFW-Dresden

Title **Spins in cages: experimental and theoretical insights into endohedral metallofullerenes' molecular magnetism**

Abstract In this talk, I will discuss recent advances in molecular magnetism research involving metallofullerenes and show how theoretical methods help assess and rationalize physical properties. In these systems, inside fullerene cages, some traditional and non-traditional atomic interactions can be realized, like single-electron $Ln-Ln$ bonds or $Ln-X-Ln$ clusters with different geometries [1-3]. Such systems often possess unique and occasionally record-breaking properties, while the complexity of chemical composition makes them challenging objects for common theoretical means. Nonetheless, modern theoretical frameworks from DFT to the *ab initio* level may help rationalize experimental outcomes in detail. I will present these advanced computational strategies that can be quite useful in describing not only Ln -based molecular but also continuous systems.

[1] Fupin Liu *et al.*, Nat. Commun. **10**, 571 (2019)

[2] Fupin Liu *et al.*, Acc. Chem. Res. **52**, 2981 (2019)

[3] Wei Yang *et al.*, Adv.Sci. **6**, 1901352 (2019)

Host: D. Inosov