

## Physics Colloquium

17<sup>th</sup> of October, 2019 at 1:00 pm  
Coffee at 12:45 pm

Campus Limpertsberg  
Bâtiment des Sciences – room BS 1.03

Talk by Prof. Stefano Vanni  
University of Fribourg, Switzerland

*Invited by Physics Research Unit.*

### Molecular simulations of biological interfaces: living dangerously out-of-equilibrium

In this colloquium, I will describe the state-of-the-art of molecular simulations of biological systems and I will present recent results from my lab showing how they have provided precise and unexpected insights into key cellular processes involving lipid membranes, including vesicular trafficking<sup>1</sup>, endocytosis<sup>2</sup> and lipid droplet biogenesis<sup>3</sup>. I will highlight how recent developments<sup>4</sup> have allowed to establish meaningful direct correlations between experimental observations and computational results, and I will discuss our efforts to develop next generation coarse-grain force fields using machine learning and biophysical experiments to address important remaining key challenges in molecular simulations of biological interfaces

1. Vanni *et al.*, Nat Comm (2014); Magdeleine *et al.*, eLife (2016); Pinot *et al.* BioRxiv (2019)
2. Pinot *et al.*, Science (2014)
3. M'Barek *et al.*, Dev Cell (2017); Zoni *et al.*, BioRxiv (2019)
4. Bacle *et al.*, Biophys J (2017); Campomanes *et al.*, Comm Chem (2019)

**Biography:** Stefano Vanni is tenured researcher at CNRS in France and Swiss National Science Foundation Associate Professor and ERC investigator in the Department of Biology of the University of Fribourg, Switzerland. His main research focus is the understanding, at the molecular level, of how emergent physical properties of biological interfaces affect intracellular trafficking and cellular metabolism.

