



Thursday, December 14<sup>th</sup>, 2017 – 02:00 p.m.  
CFEL Seminar room III (Bldg. 99)

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## Time-dependent electron-nuclear dynamics in DFTB+: theory and applications

This seminar will be focused on an implementation of electron-nuclear real-time dynamics within the Density Functional Tight-Binding (DFTB) formalism in the DFTB+ package[1], as a result of a collaboration between the Quantum Dynamics Group (University of Córdoba) and the BCCMS (University of Bremen). Some theory details will be presented as well as its application to explain the launching of mechanical oscillations in metal nanoparticles under plasmon-resonant laser illumination[2].

1. <http://www.dftbplus.org/>

2. Bonafé, F. P. et al. *Nanoscale*, 9(34), 12391–12397 (2017)

<https://doi.org/10.1039/C7NR04536K>

Host: Angel Rubio

