

Computational Materials Science@LUT

FuSuMaTech meeting December 14, 2021 Prof. Bernardo Barbiellini





High-Temperature SuperConductivity for AcceLerating the Energy Transition (CA 19108)

Collaboration with Dr. Tiina Salmi (TAU) on projects with LUT platform INERCOM.

Reserach group of Professor Bernardo Barbiellini: Toward an understanding of vortex-defect interactions

- Point-defect study: Positron annihilation spectroscopy (PAS) with DFT calculations
- The main questions to be addressed are:
 - 1) What is the highest attainable critical current Jc?
 - 2) How do we optimize vortex pinning with defects?
 - 3) What is the relationship between Jc and the point defect density?

Disorder produced by the defects, Entropy and Thermodynamics relations.

High-temperature cuprate superconductors studied by x-ray Compton scattering and positron annihilation spectroscopies <u>10.1088/1742-6596/443/1/012009</u>

Construction of HTS materials databases



Oles et al. , Condens. Matter 2019, 4, 46; doi:10.3390/condmat4020046

MATERIAL GENOME APPROACH FOR HTS: Finding new domes of superconductivity

Integrated Energy Conversion Machinery (INERCOM) LUT Platform



https://www.lut.fi/web/en/research/platforms/inercom