WP10 Data analysis Muons

Two Parma tasks
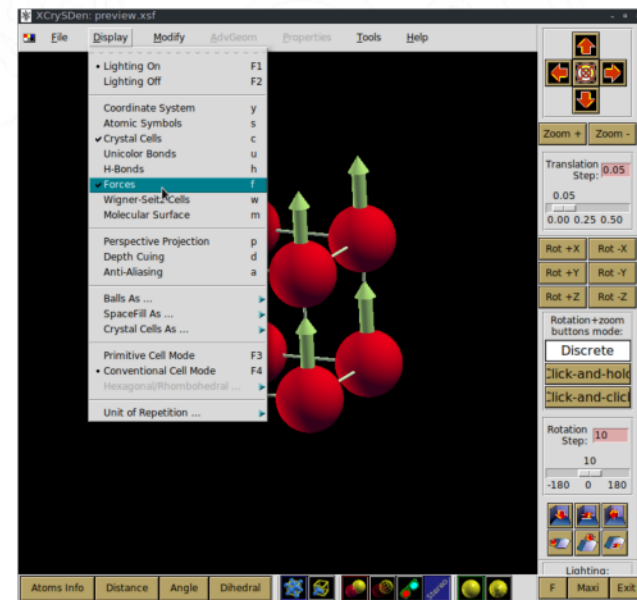
- MuESR, general purpose dipolar sum program

- Ab- initio techniques for assisting muon data analysis

IJ Onuorah, P Bonfà, RDR

DEPARTMENT OF MATHEMATICAL,
PHYSICAL & COMPUTER SCIENCES, PARMA

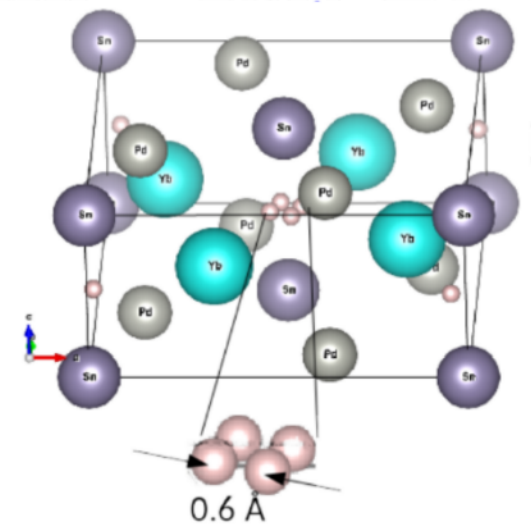# MuESR: Muon Embedding Site Refinement

- Integrated in Mantid and

- Python standalone (pip install muesr)

- General purpose: any lattice (e.g. from cif file)

- Any magnetic structure (by propagation vectors)

- Integrated visualization (VESTA or XCRYSDEN)

- Documentation on https://muesr.readthedocs

- Tutorial with several examples

- Tried out at ISIS Muon Training school with good feedback*

  * thanks A. Lim, P. Baker, C. Wilde

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DFT+Mu

0.6 Å

- Muon site determination (IJO talk)

- Muon coupling determination (IJO talk)

- Present:

  - Support of well identified experiments (1111, NiFeAs, La_2CuO_4 T', YB_2Pd_2Sn, $YBaCuFeO_5$, Sr_2RuO_4, ...

  - Textbook case exploration (e.g. fluorides, Fe, Co, Ni)

  - Muon quantum effects (with Ion Errea, San Sebastian)

- Future:

  - MD (classical vs. path integral)

  - Workflows

- PhD position available in Parma: application deadline 4 September

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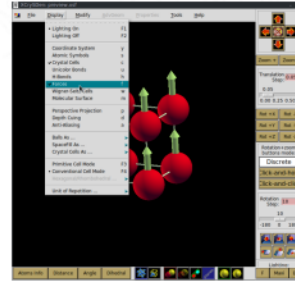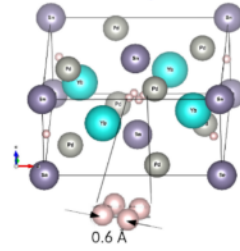
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