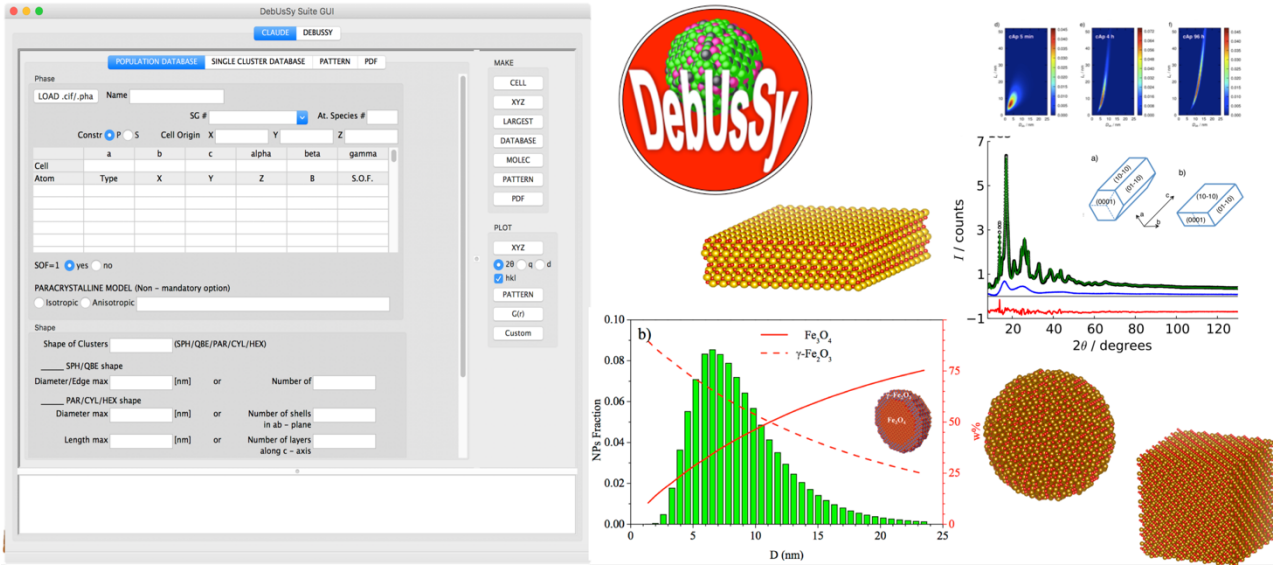
The Debussy program suite

The DebUsSy program suite (debyeusersystem.github.io) is an open-source collection of software tools implementing a fast and efficient approach to the Debye Scattering Equation (DSE) for the analysis of total scattering data in reciprocal space from nanocrystalline and/or defective materials.[1] The package consists of two main suites: *i)* **Claude** (Crystalline LAyered User DatabasE) enables users to efficiently construct atomic clusters with customizable sizes and shapes. *ii)* **Debussy** (DEBye USer SYstem) uses the databases generated by Claude to perform rapid calculations of the total scattering profiles of population of clusters contributing to the overall pattern, according to a user-defined and adjustable size-distribution function.

During the demo session, I will present a practical demonstration of key software features, including simultaneous fitting of one or multiple experimental datasets (e.g. SAXS and WAXS data, or data collected from synchrotron and laboratory instruments), analysis of single- and multi-phase samples, and modeling of structural properties (such as lattice expansion or contraction) as a function of crystal size.

This software has been successfully applied to a wide range of functional nanomaterials, including metals (also exhibiting twinning or other structural defects),[2] oxides,[3] biomimetic materials,[4] colloidal quantum dots,[5] and halide perovskite nanocrystals.[6]



[1] A. Cervellino, et al. *J. Appl. Crystallogr.* **2010**, *43*, 1543; *J. Appl. Crystallogr.* **2015**, *48*, 2026.

[2] A. Cervellino, et al. *J. Appl. Crystallogr.* **2003**, *26*, 1148; F. Bertolotti, et al. *Acta Crystallogr. A* **2016**, *72*, 632; M. Parnigotto, et al. *Small* **2025**, *21*, 2403127.

[3] R. Frison, et al. *Chem. Mater.* **2013**, *25*, 4820; F. Bertolotti, et al. *J. Phys. Chem. C* **2021**, *125*, 4806; M. Scavini, et al. *Nanomaterials* **2022**, *12*, 3385; F. Bertolotti, et al. *Nanomaterials* **2020**, *10*, 743.

[4] J. M. Delgado-López, et al. *Adv. Funct.Mater.* **2014**, *24*, 1090; F. Bertolotti, et al. *Acta Biomater.* **2021**, *120*, 167; F. Bertolotti, et al. *TrAC Trends in Analytical Chemistry* **2024**, *180*, 117904.

[5] D. Moscheni, et al. *ACS Nano* **2018**, *12*, 12558; N. Dengo, et al. *Nanomaterials* **2022**, *12*, 1252; F. Bertolotti, et al. *Nat. Mater.* **2016**, *15*, 987; L. Allara, et al. *npj Comput Mater* **2024**, *10*, 54.

[6] F. Bertolotti, et al. *ACS Nano* **2017**, *11*, 3819; F. Bertolotti, et al. *ACS Nano* **2019**, *13*, 14294; F. Bertolotti, et al. *Chem. Mater.* **2022**, *34*, 594; F. Bertolotti, et al. *Small Struct.* **2024**, *5*, 2300264.