Prof. Éric Séré  
(Université de Paris-Dauphine - FR)

will present a seminar entitled:

« The ground state of the Dirac-Fock energy »

Abstract:

“I will present a definition of the ground state for the Dirac-Fock energy inspired of Lieb’s relaxed variational principle for Hartree-Fock. This definition seems simpler and more suitable for theoretical and numerical investigations than previous ones. Based on this approach, I will present existence results for the ground state of molecules and crystals. The existence proof for this ground state suggests an algorithm for its computation, that generalizes the ODA algorithm of Cances-Lebris. The existence result for crystals is joint work with Isabelle Catto, Long Meng and Eric Paturel. The implementation and testing of the algorithm is work in progress (Guillaume Legendre, Maxime Chupin).”

Lausanne, March 22, 2024
BB/rb

Seminars are announced on the Mathematics Section website: http://memento.epfl.ch/maths/