SEMINAIRE ISMO

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Calculation of n-order derivatives of the energy in the "scc-dftb" method.

We present a method to calculate analytical n-order geometric derivatives of the energy obtained within the framework of the **self consistent Density Functional based Tight Binding approach (scc-dftb)**. In this method an expansion of the DFT Kohn-Sham integral with respect to a reference density is made. After that, a parameterization of the relevant terms is performed. The use of automatic differentiation technique allows the calculation of derivatives up to any order.

For testing the method, we calculated the energy derivatives of small and medium size systems like ethylene, benzene, naphthalene. The results showed an important improvement of calculation time and accuracy with respect to the computation of the same quantities using finite differences. Therefore, this method could be useful for spectral and dynamical calculations of bigger molecules.

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Bât. 351 - 2ème étage (Bibliothèque)

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