CONVIVIAL: a graphical user interface for performing vibrational mean field configuration interactions

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Abstract

This talk will introduce the graphical user interface called CONVIVIAL (CON-VIV Interface And Layout), for the fortran 95 code CONVIV (CONtracting VIbrations Variationally) implementing the Vibrational Mean Field Configuration Interaction (VMFCI) method. We will recall the advantages of the VMFCI method to solve the molecular vibrational Schrödinger equation, and demonstrate the functionalities of the user friendly interface CONVIVIAL.