Computational Physics Course

Learn to use software packages

In 20 December, we will learn non-adiabatic dynamics and path integral molecular dynamics.

Interested students can do the simulation using QE, but more conveniently using PIMD of Dr. Shiga
http://ccse.jaea.go.jp/ja/download/pimd/index.jp.html

PDF

Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso

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