TDAP LICENCE FOR ACADEMIC USERS

1 Motivation

TDAP ("Time Dependent Ab-initio Package") is a suite of computer software targeting for quantum dynamic simulation of electron-nuclear systems from first principles. It has been devised for general use in research practice within academic community. Some conditions have been defined for the use, distribution, and modification of TDAP, which the authors consider fair and within the common practices in academic community.

2 Definitions

Authors "The Authors" include: Sheng Meng, Institute of Physics, Chinese Academy of Sciences; Efthimios Kaxiras, Harvard University.

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1. S. Meng, E. Kaxiras. Local basis-set and real time implementation of time-dependent density-functional theory for excited state dynamics simulations. J. Chem. Phys. 129, 054110 (2008).

2. W. Ma, J. Zhang, L. Yan, Y. Jiao, Y. Gao, S. Meng. Recent progresses in real-time local-basis implementation of time dependent density functional theory for electron-nucleus dynamics. Comp. Mater. Sci. 112, 478(2016).

3. C. Lian, M.X. Guan, S.Q. Hu, J. Zhang, S. Meng. Photoexcitation in solids: First-principles quantum simulations by real-time TDDFT. Adv. Theo. Simul. 1, 1800055 (2018).

Other papers relevant to TDAP package and methods should be cited as best scientific practice dictates.

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