



Work From Home Setup Tutorial

Ryo Maezono



Work From Home Setup Tutorial:

Ab initio Calculation Tutorial Ryo Maezono, 2023-05-16 This textbook covers the framework of first principles analysis applied to materials using density functional theory DFT It provides a set of hands on tutorials using the Quantum ESPRESSO package an open source software for DFT The tutorials are well chosen designed for maximum effectiveness while requiring a minimum of the reader's time and the book describes how the essential components are combined to create the practical applications based on the idea of modeling practical problems of materials The book carefully explains how to prepare the platform to run the tutorials assisted by free software This textbook is useful for students in experimental laboratories for industrial researchers and for those not majoring in theoretical studies but learning individually

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prior knowledge of many body electron theory or simulation science Readers learn how to solve the problems on intermolecular binding forces in biomolecular systems magnetic descriptions in spintronics and material properties involving discontinuous density distributions such as surfaces interfaces and defects

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