



## Exciting Shanghai School

# Hands-on workshop on density functional theory First-principles simulations in materials science

### Organizers

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### Lecturers

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### Aims and scope

The purpose of the school is to provide an introduction to DFT for beginners (master students, PhDs, and post-docs) ranging from its theoretical foundations to practical implementations in computer softwares. In particular, the all-electron full potential augmented planewave method will be described as implemented in the **exciting** software. The necessary know-how for calculating materials properties such as structural, magnetic, linear, non-linear optical and magneto-optical properties *etc.* will be discussed through hands-on sessions and tutorials. Last but not least, an introduction to the NOMAD project, *i.e.* Novel Materials Discovery, will be given.

The School is directed to scientists in Materials Science, Physics, Electronics, Geosciences, Solid State Chemistry Physics in general, and especially to young scientists and PhD students, who wish to acquire a deep practical knowledge of state-of-the-art electronic state calculations for studying functional properties in materials science. Official language of the School is English. The school will take place in Shanghai University (Baoshan Campus).

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