

Webinar 01 — Setting the Stage (AI-generated Summary & Feedback)

1) Participation Snapshot

This first feedback webinar concludes Week 1 (“setting the stage”). Around 25 participants posted a self-presentation and joined the Zulip channels—an indication of the current cohort size. Although this run follows the synchronous track at Flemish universities, participants are geographically widespread. Compared to the original classroom audience, the course now reaches a global community.

Age distribution: about half are under 25; more than a third are 25–30; roughly one-sixth are 35–44. Backgrounds span bachelor and master students, PhD candidates, postdocs, staff scientists, industry professionals and hobby learners.

2) Expectations & Motivations

Participants rated four goals as equally important: (a) learning concepts of materials physics; (b) learning concepts of ab initio methods; (c) acquiring hands-on expertise with ab initio tools; and (d) reading papers that use such methods. Motivations include broadening one’s computational toolkit, complementing experimental profiles with computation, extending molecular simulation skills to crystalline materials, and interest in the teaching approach itself (with feedback invited via the front-page suggestion button).

3) Practical Organisation

“Weekly reports” = everything asked of you during that week (forum posts, PDFs, quizzes, and hands-on tasks). For for-credit students, completion is checked manually. Assignments include the Let’s Play (hands-on) folder, but also all other weekly tasks. Project teaming choices are collected this week.

HPC access: Flemish HPC infrastructure is accessible beyond Ghent University (ask your local HPC contacts). External volunteer learners typically cannot be granted access via the course. HPC is not required; all exercises can run on a laptop, albeit sometimes slowly. Results are equivalent regardless of machine—the difference is wall-clock time.

DFT software for projects: Quantum ESPRESSO is the default. If a team prefers another DFT code, that is acceptable—coordinate within your team (e.g., for cross-checks or to compute properties that one code handles better than another).

4) Science Highlights from Week 1

4.1 Materials “from Thought” — Reflections

Consensus has shifted: computational materials design is now widely embraced, backed by many success stories. Enthusiasm is tempered by realism—calculations are approximate and experiments remain essential. Large swaths of materials space are still unmeasured for many properties; computation helps reveal “hidden gems.” AI accelerates discovery via pattern recognition, an aspect not foreseen in older talks. Resource inequality (fast computers) influences progress, as in experimental labs, yet smart work on modest hardware remains impactful. Defects often control key properties; computations can and do treat defect physics, not just perfect crystals.

4.2 What Do We Mean by “Ab Initio”?

Ab initio models start from postulates/axioms and derive predictions mathematically (e.g., Newton’s laws, Maxwell’s equations, the postulates of quantum mechanics). Reductionism has limits: different domains demand different first-principles models; complexity can yield emergent behavior. Apply quantum methods where they make sense (e.g., everyday crystalline solids), while recognizing boundaries.

4.3 Theory, Simulation, Experiment — and Data

Theory develops equations; simulation (computer experiments) solves them—often with controlled approximations; experiment measures in the lab. A fourth pillar—data science/AI—now stands alongside the traditional triad.

4.4 Why Not “Exact” Quantum Predictions Everywhere?

We can write the exact equations (the many-body Schrödinger equation), but solving them exactly is computationally intractable. Practical methods introduce approximations to make problems solvable in human time. Quantum computing may shift the landscape someday, but useful work is already possible now.

4.5 Engineering Analogy

Bridge design uses well-validated first-principles models to build the final structure in one go. Materials discovery still relies on multiple iterations because our ab initio descriptions are approximate. That gap explains the trial-and-error character of materials breakthroughs.

5) Hardware & Software Landscape

Hardware matters because computational power doubles roughly every two years, continuously expanding what’s tractable. Keep an eye on contemporary supercomputers for perspective, even if you won’t use them directly. On software: the ecosystem is mature, with widely used atomistic codes, documentation, benchmarks, and large user communities.

6) Hands-On Setup

Install VirtualBox and import the Quantum Mobile VM to obtain Quantum ESPRESSO. Mac users on unsupported hardware can use an alternative workflow documented on Zulip; it may offer a more graphical interface. If issues arise, use Zulip first so solutions can be shared; email as a last resort.

7) Week Ahead

Begin the two-week Density Functional Theory (DFT) module—conceptual focus, not heavy mathematics. Read the project description, decide whether to participate, and fill in the form. Teams will be formed next week to start calculations.

8) Weekly Wrap-Up Activity

At the end of each session, complete a short form: (1) list the essential takeaways for the week; (2) propose an exam question. Collected takeaways and a growing bank of past and current exam-style questions will be shared under the weekly video to support your study.