

Assessment criteria

Digital Chemistry FS24 project

The project will be assessed according to the following criteria:

Methodology (30%)

- **Suitability:** The methodology chosen should be fundamentally appropriate for achieving the project's objectives.
- **Implementation:** The methodology must be implemented accurately and effectively.
- **Best practices:** The approach should adhere to the best practices as outlined in the course lectures.

Results and Analysis (15%)

- **Accuracy and reliability:** Results must be accurate and thoroughly tested for reliability. Note that the success of the project does not influence the evaluation.

Code (30%)

- **Formal criteria compliance:** The code must meet all formal requirements specified in the report outline.
- **Documentation:** An informative README file should be included, explaining the project's purpose, structure, and setup instructions. If the project is conducted on Google Colab, this can be replaced by appropriate text cells.
- **Readability and structure:** The code should be readable and well-organized, facilitating easy navigation and understanding.
- **Best coding practices:** The code should generally follow the guidelines from [PEP8](#) coding style as shown in the exercises, including appropriate documentation (docstrings and comments). [Black](#) can be used as a tool to format your code.
- **Execution:** The code should be executable without errors and the teaching team (after possible consultation with the group members) should be able to run it.
- **Performance:** The code should execute within a reasonable timeframe and reproduce the presented results accurately.

Report (15%)

- **Adherence to criteria:** The report must comply with the formal criteria outlined in the report outline.
- **Scientific language:** The use of appropriate scientific language and terminology is essential.
- **Methodology justification:** The report should clearly justify the chosen methodology and explain the reasons for not selecting alternative approaches.
- **Discussion of results:** Results should be clearly discussed, with an accurate identification of any limitations of the methods used.

Poster (10%)

- **Clarity:** The poster provides a clear overview of the project.
- **Discussion:** The students are able to explain and discuss their project in the poster session.
- **Scientific language:** The use of appropriate scientific language and terminology is essential.
- **Timely submission:** The poster is uploaded to Moodle on time.