

Faculty of Engineering

ASPIRE Summer Research Program 2026-2027

Project Title: Dielectric embedding framework for 2D materials

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Objective Implement and validate a dielectric embedding framework for 2D materials.

Project Details The dielectric embedding method is well suited for modelling large-scale structures, such as stacks of two-dimensional (2D) materials and transistor devices based on them. This approach can significantly reduce computational cost by utilising the dielectric response of individual 2D materials to construct an electrostatic model of the entire heterostructure, rather than performing expensive atomistic calculations for the full system. The project requires computing the dielectric functions of selected 2D materials using density functional theory (DFT) or tight-binding methods and employing these results within the dielectric embedding framework.

Project Timeline

TASK	1	2	3	4	5	6	7	8	9	10
<i>Literature review</i>										
<i>DFT calculations for 2D materials</i>										
<i>Dielectric function modeling</i>										
<i>Implement the dielectric embedding method</i>										
<i>Results validation</i>										
<i>Report writing</i>										

Prerequisites Python programming, basic knowledge of the density-functional theory

Student Placement Agreement

A student placement agreement must be signed by the project supervisor and the student prior to commencement of the ASPIRE program.

[LV0554-72741 ASPIRE Program Co-Curricular-Student-Placement-Agreement-Short-term.docx](#)