O.16 First-principles calculations as a backbone for the development of semiconductor technologies

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With the inherent reduction of dimensions accompanying the development of new semiconductor technologies, there is an evergrowing demand from the industry for a theoretical understanding of devices and materials at the nanoscale. First-principles calculations, especially the ones based on Density Functional Theory, can thus play a major role in the identification of new promising materials for such applications.

In this talk, we discuss how such first-principles calculations can serve as a backbone for further technological developments through several examples. This includes the prediction of new metals with competing electron-phonon and phonon-phonon contributions for thermal conductivity in the interconnect, new amorphous materials for improved thermal dissipation, and the understanding of defect formations in 2D materials which are potential candidates for the future CMOS technologies.