Theory

Current material technologies are struggling to meet the exponential growth in demand for processing power, for data transmission, and for advanced sensor technologies. This is driving the demand for new materials systems with enhanced functionality and capabilities. Major advances in device technology come both from the development of new materials systems and improved fundamental understanding. Our research in the Photonics Theory group focuses on some of the most promising emerging materials areas and device concepts for next generation devices. We target both conventional materials such as III-nitride alloys for efficient light sources as well as the investigation of metastable alloys, which combine new elements with well-established materials.

Electronic and optical properties of III-nitride alloys are significantly affected by (random) alloy fluctuations. To understand both fundamental material properties and their importance for device applications, atomistic approaches are required to provided detailed insights into phenomena related to alloy fluctuations in these systems.

Metastable group IV and III-V semiconductor alloys offer the opportunity to combine new elements with well-established materials, thereby leveraging existing mass-production approaches to enable new functionality and capabilities. Because of the chemical and size differences between the new elements and the established materials, accurate description of their electronic structure is not straightforward.

In general, our work seeks to develop and validate multiscale models for their electronic and optical properties, and then to apply those models, in collaboration with leading experimental groups and industry partners, to demonstrate the potential of these alloys for future device applications.
Localised indium state above the conduction band edge in Al\(_{1-x}\)In\(_x\)N.

With group IV semiconductors, we target direct gap alloys (SiGeSn, Ge:C) for:

- future tunnelling field effect transistor devices and viable group IV optical sources, and
- suitable SiGeSn alloys for incorporation in high efficiency multijunction solar cells.

With III-V semiconductors, we have shown that bismuth-containing alloys open wide opportunity for band structure engineering in photonic devices; our research targets their potential to dramatically improve photovoltaic efficiency and to provide dramatically improved optical sources and detectors for sensing and diagnostics.

Overall, we are one of the few groups worldwide which have the aim and capability to start from first principles investigations of fundamental processes and carry through to investigations that guide and lead the development of electronic and photonic devices with enhanced capability and functionality.

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Related Publications

- Optical gain in GaAsBi/GaAs quantum well diode lasers
  Scientific Reports volume 6 issue 1 (2016)
  Authors: Igor P. Marko, Christopher A. Broderick, Shirong Jin, Peter Ludewig, Wolfgang Stolz, Kerstin Volz, Judy M. Rorison, Eoin P. O’Reilly, Stephen J. Sweeney

- Impact of cation-based localized electronic states on the conduction and valence band structure of Al1−xInxN alloys
  Authors: S. Schulz, M. A. Caro, E. P. O'Reilly

- Theory of local electric polarization and its relation to internal strain: Impact on polarization potential and electronic properties of group-III nitrides
  Authors: Miguel A. Caro, Stefan Schulz, Eoin P. O’Reilly

- Tight-binding analysis of the electronic structure of dilute bismide alloys of GaP and GaAs
  Physical Review B volume 84 issue 24 (2011)
  Authors: Muhammad Usman, Christopher A. Broderick, Andrew Lindsay, Eoin P. O’Reilly