

# ***Ab initio* prediction of the electronic and optical properties of single-walled GaN nanotubes**

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Gallium nitride is a key material in optoelectronics. Recent efforts have focussed on growing GaN nanostructures in order to engineer their electronic properties. To date, the main focus has been on nanowires, but there is ongoing interest in creating and studying nanotubes.

I present first principles results for the electronic and optical properties of isolated single-walled GaN nanotubes. I employ *ab initio* Green's function methods: the *GW* approximation for the electron self-energy and the Bethe-Salpeter Equation (BSE) for excitonic effects. The method uses periodic supercells, so it is necessary to truncate the Coulomb interaction properly in order to avoid artificial periodic image interactions. I outline a recently developed general approach for such truncations.<sup>1</sup>

- [1] S. Ismail-Beigi, "Truncation of periodic image interactions for confined systems", in press at *Physical Review B* (2006); preprint available on <http://www.arxiv.org/abs/cond-mat/0603448>