

Abstract Submitted
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Second Harmonic Generation of Transition Metal Dichalcogenides from First-Principles.¹ MICHAEL LUCKING, HUMBERTO TERRONES , Rensselaer Polytechnic Institute — The monolayers of transition metal dichalcogenides (TMDs) have been observed to have strong non-linear optical properties. We present calculations of the second harmonic generation (SHG) of nanostructured TMDs. In particular, the zigzag nanotubes exhibit a strong enhancement in the second harmonic signal. However, the armchair nanotubes have no second harmonic signal, making SHG an efficient tool for determining the chirality of grown nanotubes.

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Michael Lucking
Rensselaer Polytechnic Institute

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