Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Computational and Experimental Design of Functional Deep-Ultraviolet Non-Linear Optical Materials JOSHUA YOUNG[1], Drexel University, JAMES RONDINELLI, Northwestern University, HONGWEI YU, HONGPING WU, WEIGUO ZHANG, P. SHIV HALASYAMANI, University of Houston — Non-linear optical (NLO) materials are of intense interest owing to their ability to generate coherent radiation at a variety of difficult to access wavelengths. However, designing materials to access the deep ultraviolet (DUV, $\lambda < 200$ nm) region remains a significant challenge, as such a compound must exhibit a number of characteristics including a non-centrosymmetric crystal structure, wide band gap ($E_g > 6.2$ eV), large second harmonic generation (SHG) coefficients, and moderate birefringence. In this work, we use first-principles density functional theory calculations and introduce new structural metrics to disentangle the contributions of crystal-chemistry and NLO-active structural units to the properties of several newly synthesized DUV NLO materials. We find that the presence of stereo-active lone pair cations (such as Pb^{2+}) and triply bidentate cations enhance the SHG response, while polyhedral units serve to lift inversion symmetry in the crystal structures. We anticipate that the targeted design approach applied here can be harnessed for the discovery of advanced optical materials at other important regions of the electromagnetic spectrum.

[1]Current affiliation: Naval Research Laboratory

Joshua Young
Naval Research Laboratory

Date submitted: 11 Nov 2016 Electronic form version 1.4