Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**Excitonic states and defect physics of two-dimensional group-IV monochalcogenides.**[1] LIDIA GOMES, ALEXANDRA CARVALHO, PAOLO TREVISANUTTO, ALEKSANDR RODIN, ANTONIO NETO, Centre for Advanced 2D Materials and Graphene Research Centre — Layered group-IV monochalcogenides have become an important group of materials within the ever-growing family of two-dimensional crystals. Among the binary IV-VI compounds, SnS, SnSe, GeS, and GeSe form a subgroup with orthorhombic structure which has shown exciting particularities and has been considered of high potential for numerous application. We give a brief overview of some important properties of the 2D form of this group and focus on recent results addressing the excitonic properties and the impact of the introduction of point defects on their structures. Vacancies and oxygen defects are modeled using first principles calculations. Energetic and structural analysis of five different models for chemisorbed oxygen atoms, reveals a better resistance of these materials to oxidation if compared to their isostructural partner, phosphorene. We also discuss a parallel work where quasi-particle band structure and excitonic properties of GeS and GeSe monolayers are investigated through ab initio GW and Bethe-Salpeter equation calculations. Within the main results, we show that the optical spectra of both materials are dominated by excitonic effects, however, GeS presents a remarkably larger binding energy of 1 eV.

[1]NRF-CRP award Novel 2D materials with tailored properties: beyond graphene (R-144-000-295-281) 1

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Date submitted: 11 Nov 2016 Electronic form version 1.4