XII th Biennial National Conference of
Physics Academy of North East (PANE2021)
Organized by Department of Physics, Tripura University
15 - 17 December, 2021

Title of the work:

Effects of doping of zinc and mercury composition-dependent opto-electronic properties of $Cd_{1-x-y}Zn_xHg_yS$ quaternary alloys: A First-principles investigation

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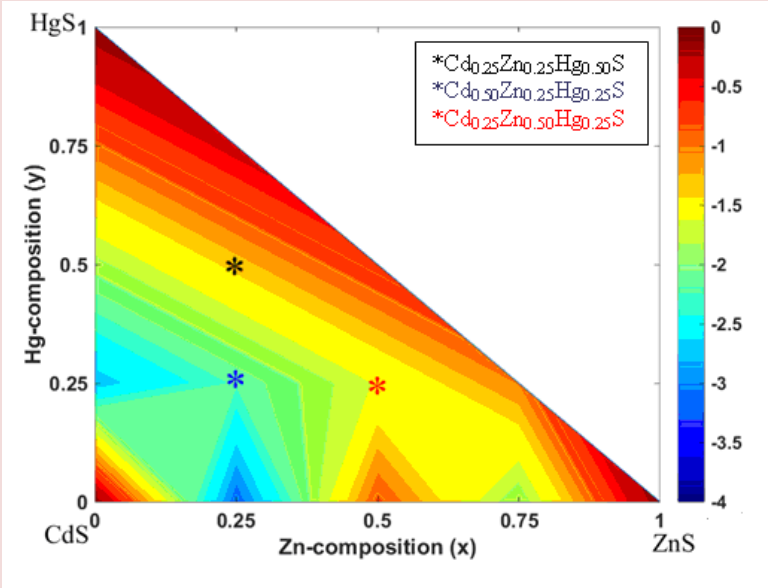
Objectives of the work:

- The zinc and mercury composition dependence of various physical properties of triangular $Cd_{1-x-y}Zn_xHg_yS$ quaternary alloys.
- DFT oriented FP-LAPW approach in association with PBE-GGA, mBJ-GGA, and GGA+U exchange-correlation potential schemes have been used.
- To investigate the practical usage of the mentioned quaternary alloys.



- Calculated negative formation energy ensures that each quaternary alloy is thermodynamically stable.

Observation and Result:

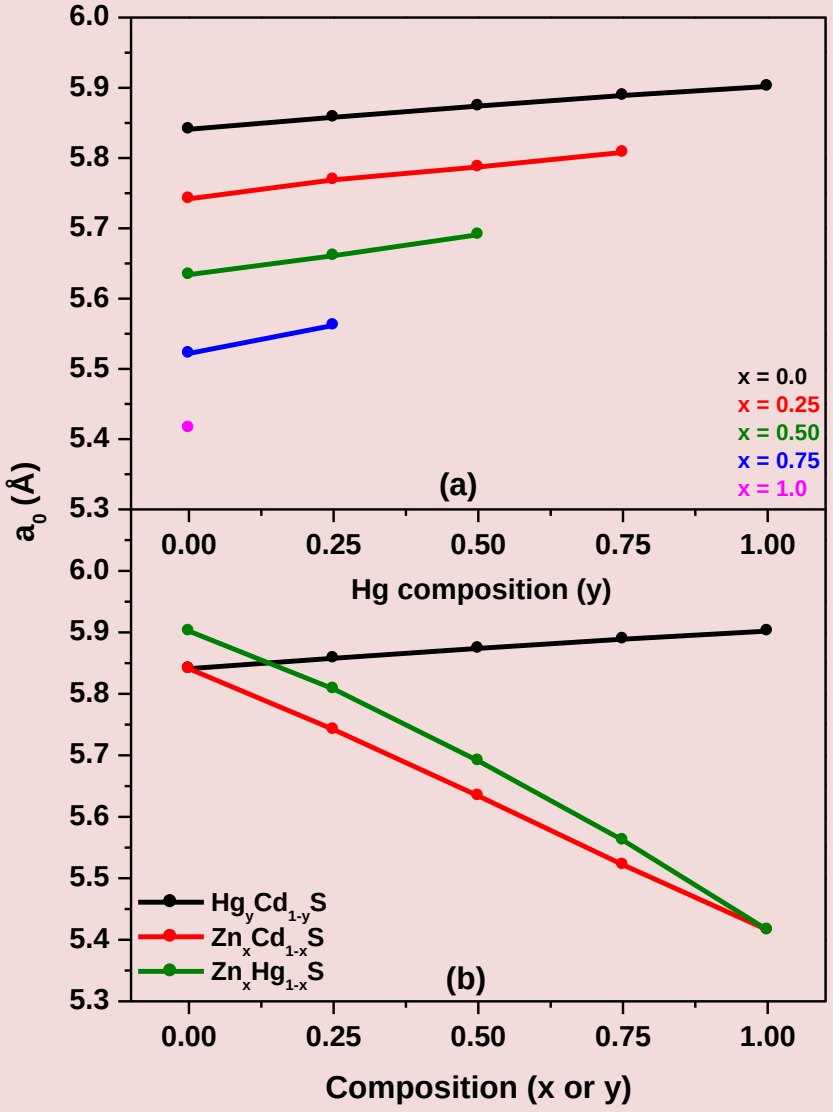
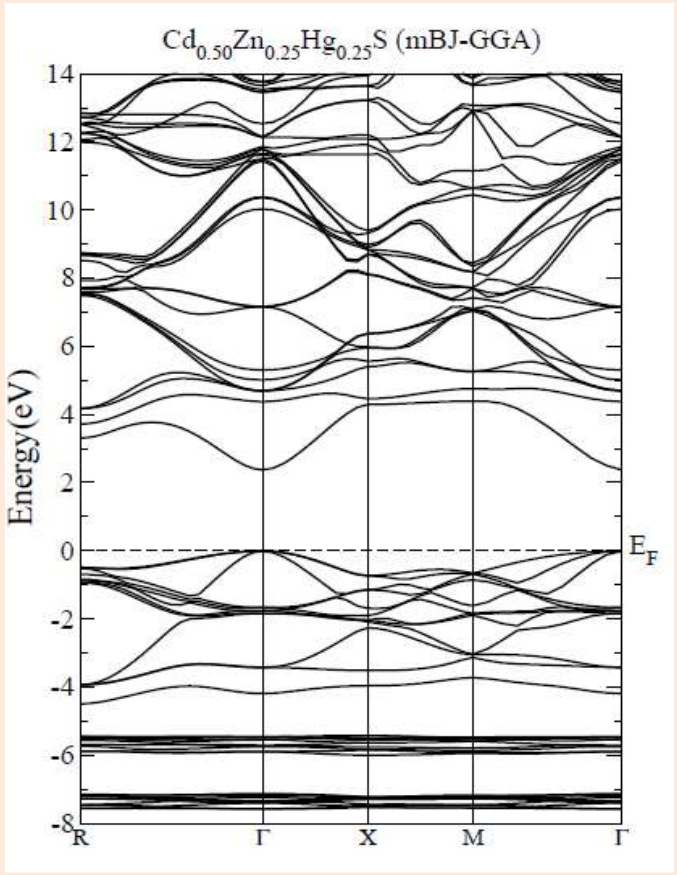
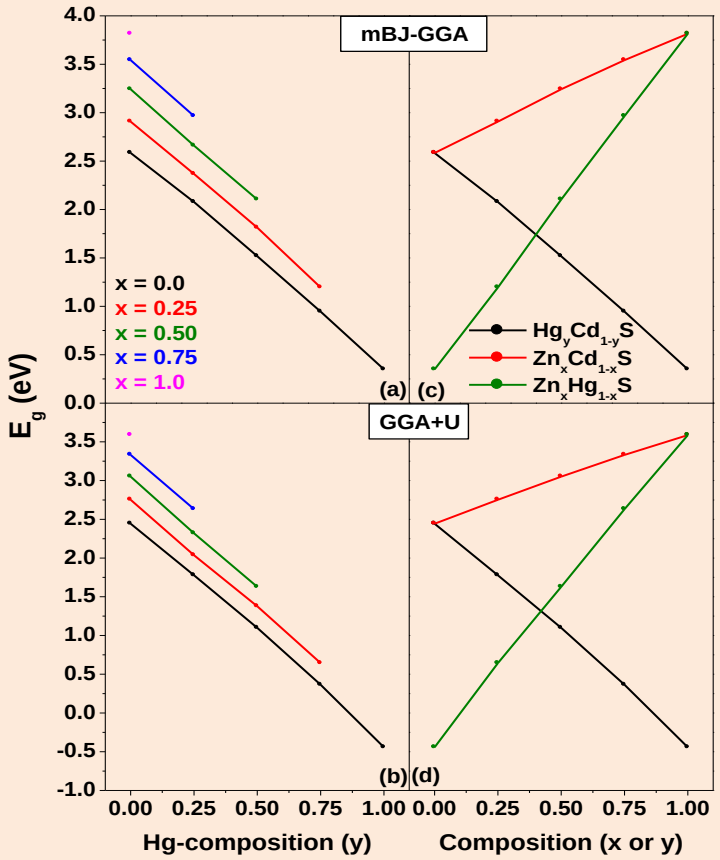
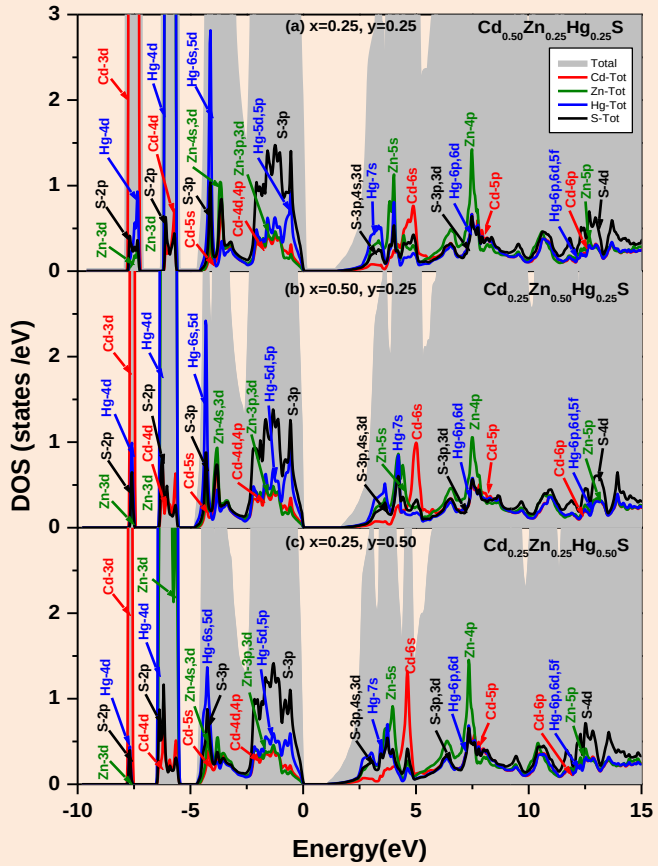


Figure 1

Electronic Characteristics and Density of State (DOS)

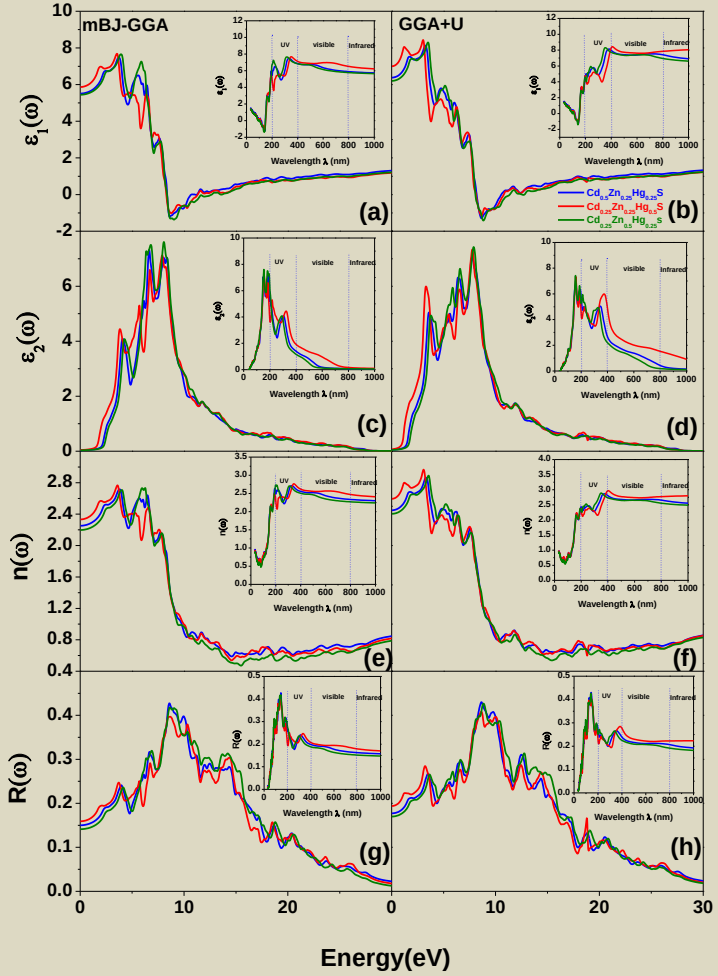


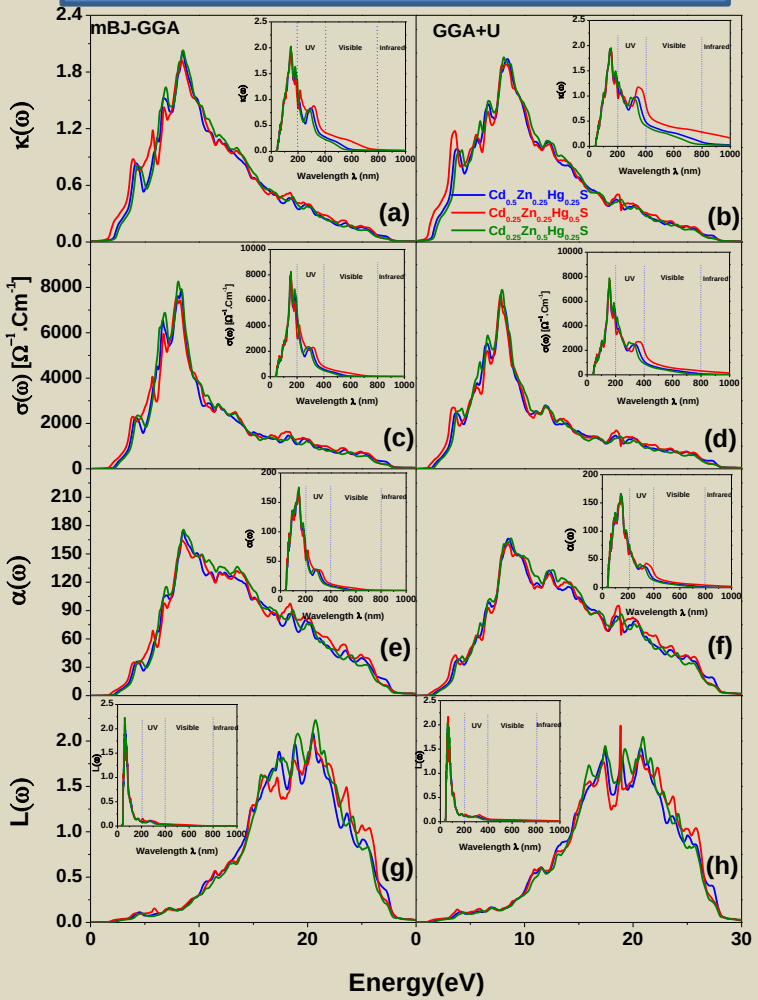


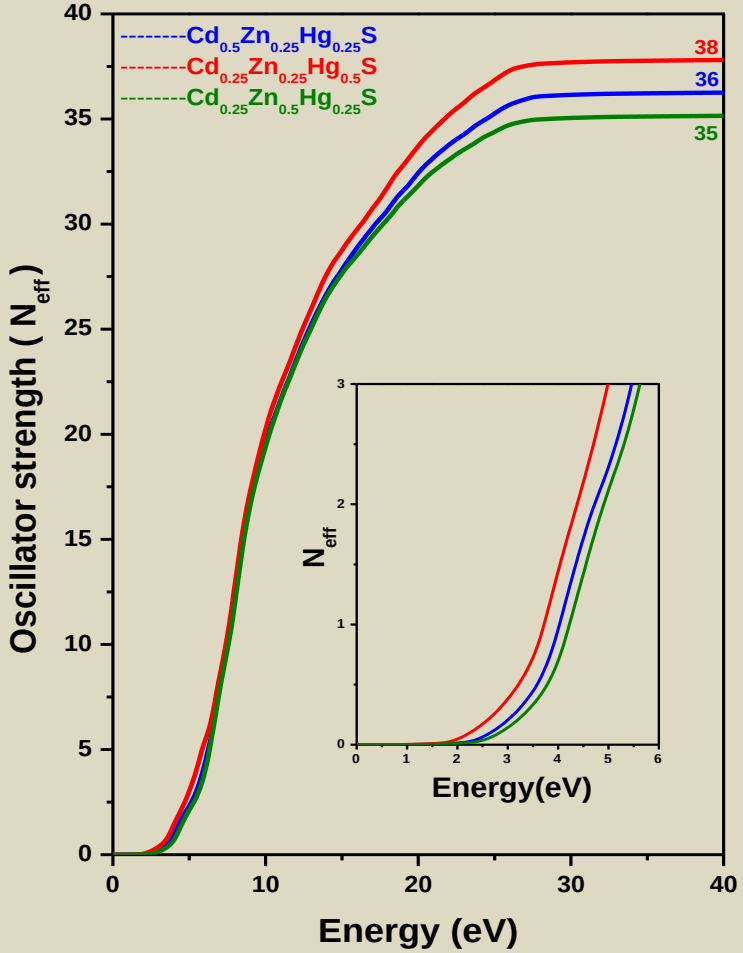


- Calculations with mBJ-GGA potential scheme show that all the specimens are direct band gap (Γ–Γ) semiconductors. Though calculations with GGA+U potential scheme, only HgS shows the metallic character with negative fundamental band gap and it follows the corresponding experimental investigations.
- Electrons play dominant role over holes in carrier transportation due to their much lower effective mass compared to holes.
- Exclusive or collective contribution of electronic excitations from occupied S-3p valence state to unoccupied Zn-5s, Cd-6s, and Hg-7s conduction states are observed from DOS.

Optical Characteristics







- At incident energy = E_g, interaction between electrons and incident photon has been initiated and electrons start arriving at the unoccupied states of the CB.
- Each of these numbers is the signature of maximum oscillator strength that the corresponding quaternary alloy is able to exhibit.

- Absorption of any of these quaternary alloys is significantly large in the high energy region compared to reflection and transmission. Transmission of any quaternary alloy is significantly high in extremely low energy region compared to reflection and absorption.

Conclusion and Discussion :

- **The ternary and quaternary alloys under the $Cd_{1-x-y}Zn_xHg_yS$ system are zinc-blend crystalline direct band gap (Γ-Γ) semiconductors.**
- **Their optical properties depend on Γ-centered direct band gap.**
- **In these specimens, carrier transportation mainly due to electrons causes high electron mobility in these specimens.**
- **Suitable for preparing luminescent device due to their substantially high luminescence efficiency.**
- **Potential materials for high quality cladding in quantum well structures by precisely controlling their compositions and hence lattice constant and band gaps.**
- **These materials are also well suited for preparing UVA detectors as well as materials of interest for UV optoelectronics.**


Thank You