**Deep Acceptor Polarons in a-TeO2 and Hydrogen-induced Instabilities in IGZO**

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The talk is in two parts. There is a lack of p-doped amorphous semiconductors with moderate deposition temperature for back-end of line (BEOL) semiconductor processing. Undoped 𝛽-TeO2 is a high mobility p-type semiconductor1. However, there has been no experimental proof that p-type doping leads to conductive acceptor states, as EF of undoped a-TeO2 lies near midgap2. Recent GGA studies on AsTe sites found shallow p-type states3, but the unit cell was too small. Larger 216-atom cells using hybrid HSE functionals presented here find deep states, Fig. 1. The acceptors form deep, non-doping configurations with angular polaronic distortions (Fig. 2) with broken As-O bonds. This is more complex than simpler vacancy defects4, Fig 2. The band edge energies fall outside the limits for doping3,4. The distortions arise because the network has a low mean coordination of 2.4, the floppy limit for such lattices5.

We also study hydrogen-induced instabilities in the n-type InGaZn oxide semiconductor, of major technological interest for BEOL processing. Some Metal-H and oxygen-H configure-ations proposed in Bang6 are evaluated using GGA+U and HSE calculations, Fig. 3.

1. A Zavabeti, et al, Nature Electronics **4** 277 (2021)
2. J Shi, .. K H L Zhang, App Phys Lett **122** 101901 (2022)
3. J Robertson et al, App Phys Lett **124** 212 101 (2024)
4. Z Xiao.., H Hosono, Chinese Physics Lett **42** 016103 (2025)
5. H He, M F Thorpe, Phys Rev Lett **54** 2107 (1985)
6. J Bang, S Matsuishi, H Hosono, APL 110 232105 (2017)

A graph of energy

Description automatically generatedA close-up of a molecule

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Fig. 3 Partial density of states of M-H and M-OH configurations in amorphous IGZO.

Fig. 2 Atomic structure and localised acceptor state of AsTe.

Fig. 1. GGA, green dots. HSE, red dots for various p-dopant sites.