



Contribution ID: 9

Type: **Oral Presentation**

On the orbital rehybridization in tetrahedral amorphous carbon

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The use of tetrahedral amorphous carbon thin films in bolometers depends strongly on the ability to tune its optical properties. This can be achieved by controlling the density of dangling bond defects and the disorder in the material. The pi-orbital axis vector theory is used in this study to investigate the phenomenon of rehybridization of the carbon bonding in tetrahedral amorphous carbon. It is shown that the correlated pi - pi* orbitals is locally entangled due to the competition between the on-site Coulomb interaction and the hybridization. A microscopic model is proposed for the reduction in strain in the material due to hydrogenation, based on the the sp³ – sp² conversion reaction. It is demonstrated that the activation energy for this conversion is dependent on the Urbach energy, and therefore on the disorder. The implication of the results on the manifestation of strain in similar, carbon-based, materials is discussed.

**Level (Hons, MSc,
 PhD, other)?**

Other

**Consider for a student
 award (Yes / No)?**

No

**Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?**

Yes

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