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## STRUCTURE-AMMONIA SENSING PROPERTY CORRELATION IN $\text{Sn}_{1-x}\text{V}_x\text{O}_2$ MESOPOROUS NANOPARTICLES

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Doping is a well-known method for improving gas sensing responses by metal oxide based functional materials.[1] And the plausible explanations provided in justification of using a specific dopant have been changes in material crystallinity, particle size, morphology and so on; but these ideas alone aren't able to clearly highlight the fundamental changes and intricacies of a system that exhibits improved performance by virtue of doping.[2] In this context, we have tried to analyze improved ammonia sensing responses by vanadium doped tin oxide nano-particles of formula  $\text{Sn}_{1-x}\text{V}_x\text{O}_2$  with respect to crystal structure and surface structural aspects.[3] While the doped samples showed a nearly four-fold improved response as compared to pure  $\text{SnO}_2$ , the sample  $\text{Sn}_{0.696}\text{V}_{0.304}\text{O}_2$  showed 1.2 times improved response than  $\text{Sn}_{0.857}\text{V}_{0.343}\text{O}_2$ . Structural analyses by Rietveld refinement[4] revealed reduction of unit cell volume in doped samples, leading to generation of surface active sites up to  $1019/\text{mm}^3$  of doped sample, explaining improved response by increase in surface interaction. Surface structure analyses by XPS reveal presence of 1.2 times excess surface positive charge in  $\text{Sn}_{0.857}\text{V}_{0.343}\text{O}_2$  as compared to  $\text{Sn}_{0.696}\text{V}_{0.304}\text{O}_2$ . Considering the concept of charge immobilization by surface electronic states in the former, the variable sensing responses amidst the doped samples can be explained. The specific role of vanadium ion in improving ammonia sensing responses by pure  $\text{SnO}_2$  has been delineated.

References:

- [1] Morrison, S. R. Mechanism of Semiconductor Gas Sensor Operation Sensors and Actuators 1987, 11, 283 – 287.
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- [3] Rietveld, M. H. A profile refinement method for nuclear and magnetic structures J. Appl. Crystallogr. 1969, 2, 65-71.
- [4] N. Chakraborty, A. Sanyal, S. Das, D. Saha, S. K. Medda and S. Mondal, Ammonia Sensing by  $\text{Sn}_{1-x}\text{V}_x\text{O}_2$  Mesoporous Nanoparticles, ACS Appl. Nano Mater. 2020, 3, 8, 7572-7579.

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