



## **Research Papers**

### **Self-diffusion of lignite/water under different temperatures and pressure: A molecular dynamics study**

*Xinjian Liu, Yu Jin, Congliang Huang, Jingfeng He, Zhonghao Rao, Yuemin Zhao*  
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### **Optical properties of pure and TM-doped single-walled ZnO nanotubes (8,0) (TM = V and Co) by first principles calculations**

*R. Taghavi Mendi, M. Majidiyan Sarmazdeh, A. Boochani, S. M. Elahi, S. Naderi*  
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*Rashid Ali, H. A. Shah*  
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*Bo Wang, Hongtao Li, Wenhao Shu, Wenhua Li, Li Chen, Liang Lei, Jinyun Zhou*  
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*Mehrdad Moradi, Majid Ghanaatshoar*  
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*Minjie Wang, Caiwen Ma*  
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*Shuo Zhang, Yongguang Yu, Guoguang Wen, Ahmed Rahmani*

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*Lei Wang, Feng-Hua Qi, Bing Tang, Yu-Ying Shi*

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**Electronic structure, magnetism and stability of  $\text{Co}_2\text{CrX}$  ( $X=\text{Al, Ga, In}$ ) *ab initio* study**

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