

# Gemeinsames Kolloquium der Sonderforschungsbereiche 445, 491 und 616

Vortragender: **Dr. Vijay Kumar**

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Gast von Prof. Entel

Thema: **Ab initio design of novel nanomaterials using doping and nanocoating**

Abstract: Doping of bulk materials is very important to produce semiconductors for devices, improved steels, optical materials and other applications while coating is important for protection, catalysis, optical and magnetic applications to name a few. Nanomaterials are currently attracting great interest and at the nanoscale doping could lead to novel atomic structures as well as new properties and applications. We have used doping of metal atoms in semiconductors such as Si to predict from *ab initio* calculations the formation of silicon fullerenes and other polyhedral as well as tubular forms [1] that have been subsequently produced in laboratory while doping of gold clusters has been used to make multifunctional magnetic clusters of gold [2] that have potential for applications in imaging and cancer therapy. Most recently we have used doping to make graphene semiconducting [3]. On the other hand coating of nanoparticles is a necessity in some cases to protect their properties and it is also used to make novel core shell structures. I shall discuss the formation of 14 carat Al-Au fullerenes that were predicted [4] from coating of a gold layer on an aluminum cluster and some results on the passivation of II-VI semiconductor quantum dots as well as their doping with magnetic atoms [5].

[1] V. Kumar and Y. Kawazoe, Phys. Rev. Lett. **87**, 045503 (2001); *Nanosilicon*, (ed.) V. Kumar, Elsevier (2008); V. Kumar, Comp. Mater. Sci. **36**, 1 (2006).

[2] B.D. Yadav and V. Kumar, Appl. Phys. Lett. **97**, 133701 (2010).

[3] P.P. Shinde and V. Kumar, to be published.

[4] V. Kumar, Phys. Rev. B **79**, 085423 (2009).

[5] S.P. Nanavati, V. Sundararajan, S. Mahamuni, V. Kumar, and S. V. Ghaisas, Phys. Rev. B **80**, 245417 (2009).

Zeit: **Donnerstag, 16. Juni 2011, 16:00 Uhr**

Ort: **Gebäude MD, Raum 349** (Campus Duisburg)  
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Interessenten sind herzlich willkommen

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Prof. Dr. Dr. h. c. H. Zabel  
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Prof. Dr. M. Horn-von Hoegen  
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