

Laboratory Name: Idaho National Laboratory
B&R Code: KC0202030

FWP Title: Structural and Electrostatic Effects in Self Assembled Nanostructure and Interface Growth.
FWP Number: 1147 (101319)

Program Abstract: This basic research Task, outlined in the following, is focused on obtaining a better understanding of nanoparticles, surfaces and of interfaces. Such an understanding of the interfaces between nanostructures and their substrates, and between heteroepitaxied materials, is of considerable interest both in terms of increasing our fundamental knowledge and of facilitating our ability to synthesize these important systems. The primary approach used in this work is the comparison of experimental data with model calculations, and the use of model calculations to explore new systems for which detailed experimental data is not available. Theoretical studies will use first-principles, density functional theory calculations and other formalisms.

Program Impact: The work performed under this task is designed to increase our understanding of the forces that shape the detailed atomic nature of surfaces and interfaces under both equilibrium and non-equilibrium conditions in a wide variety of systems of importance to DOE's missions.

FY 2009 Authorized Budget (New BA):

FY09 BA \$200K

FY10 BA \$200K

FY11 BA \$0K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE

Helen H. Farrell, Principal Investigator, 40%.

Interactions: Idaho National Laboratory (C. D. Van Siclen, D. M. Ginosar, L. M. Petkovic, S. Rashkeev); University of California at Santa Barbara (C. J. Palmstrom); Cornell University (Darrell Schlom).

FY 2009 Major Program Achievements:

Despite the fact that FY2009 was an extremely challenging year due to the necessity of being on both short term and long term leave due to medical reasons, significant progress was made in this program. Three papers were published in 2009 that were funded at least in part by this FWP. These are listed in the section under published papers. In addition, another paper, "Effects on the constituent properties of nanoparticles," with Petkovic and Ginosar, was begun. Of the five oral presentations and posters that were presented at professional meetings, the three most heavily dependent upon funding from this FWP were:

1) H. H. Farrell*, B. D. Schultz and C. J. Palmstrom, "The GaAs(111)B surface revisited", The XXXVI Physics and Chemistry of Surfaces Meeting, Santa Barbara, CA, January, 2009.

2) H. H. Farrell*, R. D. Parra, L. M. Petkovic, D. M. Ginosar and C. D. Van Siclen "Effects on the constituent properties of nanoparticles," 2009 Villa Conference on Interactions Among Nanostructures, St. Thomas, U.S. Virgin Islands, September 6-11, 2009.

3) H.H. Farrell*, L.M. Petkovic, D.M. Ginosar, "Considerations for catalyst properties required for S-I thermochemical cycle applications," 237th ACS National Meeting & Exposition, March 22-26, 2009, Salt Lake City, UT. (FUEL Division). Published in meeting proceedings.

FY 2009 Recognition, Honors, and Awards: in FY2009, Farrell became INL Directorate Fellow.

FY 2009 Journal Publications: 1) R. D. Parra and H. H. Farrell, "Binding Energy of Metal Oxide Nanoparticles", J. of Phys. Chem., C, **113**, 4786, 2009.

2) H. H. Farrell, B. D. Schultz*, C. J. Palmstrom*, "Comment on 'High-resolution core-level photoemission study on GaAs(111)B surfaces' [J. Appl. Phys. 101, 043516 (2007)]", J. of Appl. Physics, **105**, 056106 (2009). { * ONR funding for Schultz and Palmstrom }

3) S. N. Rashkeev**, D. M. Ginosar*, L. M. Petkovic*, H. H. Farrell, "Catalytic activity of supported metal particles for sulfuric acid decomposition reaction," Catalysis Today 139 (2009) 291-298. { *LDRD and Nuclear Hydrogen funding for Petkovic and Ginosar, ** internal INL funding for Rashkeev. }