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Biocomplexity Faculty Search Committee
C/O Prof. Rob de Ruyter van Steveninck
Biocomplexity Insititute
Indiana University
Swain Hall West 117
Bloomington, IN 47405-7105
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Dear Professor Rob de Ruyter van Steveninck:

It is with great pleasure that I recommend Dr. Rahul V. Kulkarni for a faculty position in your department. I have known Dr. Kulkarni for approximately eight years now, first as a bright eyed and enthusiastic student in my Many Body Theory class at Ohio State University. I was so impressed with Rahul and his progress that I hired him as a postdoctoral researcher some time after I moved to UC Davis, and I was very happy with my decision. Rahul is an exceptionally broad, nimble, and enthusiastic young theoretical physicist who has the potential to become a leader in the field of biological physics. I think he is exceptionally well suited as a candidate for your position.

Rahul has done work with me in two main areas: first, he has been a very significant collaborator in the group of Rajiv Singh and I studying aggregation phenomena in amyloid diseases, especially prion diseases. In this work we have developed a cellular automata model to capture the essential features of incubation time statistics and a possible treatment protocol for the disease. Rahul has participated in three publications in this area (in Physical Review Letters and Biophysical Journal), and we have invited him to give a talk at an upcoming workshop on molecular level studies of amyloid disease we are co-organizing (http://sexton.ucdavis.edu/icamyloid.html).
On the first paper, Rahul participated heavily in the analysis of simulation data generated as part of Alex Slepoy's dissertation work. On this second, Rahul has been the real leader. He has not only developed very complete analytic treatments to approximate our cellular automata simulations, he has also carried out detailed data analysis, and plunged with great alacrity into the prion disease literature coming out with gem after gem of phenomenological insight. Indeed, he became a practical walking encyclopedia of prion data, one to consult with all questions! He took the

primary role in writing up our work and shepherding it to submission. He gave a splendid invited talk two years ago at the APS March meeting on our work.

Second, he has worked with my students and I on developing combined first principles (density functional theory) and many body modeling of the biomimetic cobalt valence tautomer molecules, which may also be useful in magnetic switching devices. Moreover, they are potential models for spin crossover complexes in metalloproteins and metalloenzymes with transition metal ions. Being novices in the use of density functional theory, my group relied on Rahul's expertise to get the SIESTA code (provided to us by Prof. P. Ordejon) up and running. These molecules are mysterious. There is an entropy driven transition at which the magnetic moment `collapses' concomitant with a collapse of the octahedral coordination sphere around the central cobalt ion (bond lengths decrease by 10%). Experimentally inferred entropy and enthalpy changes (derived from fits to the magnetic susceptibility) suggest enormous values (an entropy change of 10-15k_B, and an enthalpy change of around 0.3 eV/molecule!). On the other hand, a direct heat capacity measurement gives values one order of magnitude smaller. Rahul showed that a fully relaxed density functional theory treatment of the high temperature state and low temperature state reduced previous estimates of the enthalpy by 0.6 eV per molecule (electron correlations seem to get the rest of it!), and that a finite size broadened first order phase transition explains the magnitude of the entropy/enthalpy changes (the molecules cluster in either solution or molecular solid form). We hope to move from this work to other less well-understood tautomer molecules, and to modeling the transition metal prosthetic complexes in proteins and enzymes.

In addition, Rahul continued his very nice work on small world networks and fractional superconducting vortices while at Davis, striking up his own collaborations elsewhere. The latter work is characteristic of Rahul's style: with a clever insight, he produced a variational theory of the fractional vortices, which agrees extraordinarily well with simulations. Recently he has found ways to generalize this effort to 1D problems. He has given two invited talks at local meetings about the fractional vortex work. I have also been very impressed with his dissertation work on surface reconstruction phenomena using density functional theory, which apparently has led to some re-evaluation of experimental data.

Recently, he has been doing what looks like some strong bioinformatics work, but Ned Wingreen will be able to tell you more about that in detail.

In addition to his clear scientific talent, Rahul has an infectious enthusiasm for physics, excellent communication skills, and a great taste for tackling problems, which are doable in a finite time scale, yet important.

Rahul is comparable in talent to some other recent postdocs. He is somewhat below Gergely Zarand at a comparable age, but Gergely was recently named top young scientist in Hungary (he is a professor at the Technical University of Budapest). He is comparable in intellect and accomplishment at this stage to Avi Schiller (now a professor of physics at the Hebrew University of Jerusalem

Rahul's excellent communication skills and enthusiastic approach to science bode well for his development as a teacher and mentor. His great interest in interdisciplinary problems and collaboration will position him well in this emerging era of group-oriented grants.

In short, Rahul V. Kulkarni is broad and deep scientist, very capable both in analytic theory and in computational physics. He wants to continue working on biologically motivated physics, and I think he would be a fine candidate for your position.

If I can be of further assistance, don't hesitate to contact me.

Sincerely,

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