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Prof. Dr. Nicola Spaldin  
Materials Theory  
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Dear Dr. Spaldin,

I am writing this letter in response to the advertisement seeking applicants for a PhD position on “Advanced Electronic Structure Methods for defects in transition-metal oxides (Project C)” in the Materials Theory Division, Department of Materials, ETH Zurich. Presently, I am working as a project engineer in the Indian Institute of Technology Kanpur, from where I completed my master-level study (June, 2015) in materials science, under the valuable guidance of Dr. Somnath Bhowmick, Dr. Anshu Gaur and Dr. Amit Agarwal. Being familiar with the diverse fields of materials physics, I am aware of how crucial the described project is, both to fundamental theory and to the emerging technologies. I sincerely believe that I could undertake this ambitious opportunity, due to my two years of experience in the electronic structure of materials (using first-principles techniques), along with my academic excellence (CPI 9.5/10) in subjects relevant to the project description.

In my postgraduate thesis work, we introduced evolutionary algorithms (together with DFT) to predict the structure of amorphous materials from first-principles ([arXiv:1605.00516](#)). This methodology follows a non-local temperature independent route, to predict the local structure of amorphous materials and excels in many aspects over the conventionally adopted techniques. Following this, I got involved in two additional project works, both of which were related to the study of external perturbations on the electronic structure of low dimensional materials. In the first work ([Phys. Rev. B 91, 115433](#)), we predicted a “semiconductor to metallic transition” in blue phosphorene at high electric fields and in the other work ([Phys. Rev. B 93, 165413](#)), we observed noticeable variations in the electronic and transport properties of black phosphorene under controlled chemical functionalization (using cluster expansion technique with DFT).

Working in distinct domains of materials physics (within the framework of DFT) has been quite a gratifying experience to me. However, currently I would like to become more focussed and work specifically on the physics of “strongly correlated materials”, particularly transition metal oxides (TMOs) using post-DFT methods (DMFT, DFT+U, GW etc.). This specific interest in TMOs, above all is due to the numerous electronic phases emerging out of the interplay between strong polarizability of metal-oxide bonds and the electron-electron correlations in these materials.

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Now that I am eagerly looking forward to my doctoral studies to pursue my goal of a research oriented career and delve deeper into the physics of *strongly correlated materials*, the advertised doctoral position seems like a perfect opportunity for fulfilling my research objectives. By going through your article published in Science magazine titled “Functional Ion Defects in Transition Metal Oxides (2013)”, I learned that defects, like other external fields (electric, magnetic and stress) could actively control the functionality of TMOs, leading to a plethora of novel research possibilities. Thus, I expect to encounter plenty of exciting phenomena while trying to study the interplay of defect chemistry, epitaxial strain and functionality in TMOs as mentioned in the project statement. My familiarity with the effects of such perturbations on the electronic structure of a material and my basic programming skill sets (Fortran, Python, Shell-scripting etc.), both of which are pertinent to the project description, will definitely assist me to begin my work with great momentum, if selected.

I am enclosing my curriculum vitae for your consideration. Kindly notify me, if there are any other materials or information required, that will assist you in processing my application. I remain at your disposal for any further information you may require or an eventual interview.

Thank you for your kind consideration. I look forward to hearing from you.

Yours sincerely,

A handwritten signature in black ink, appearing to read 'Suhas Nahas', written over a diagonal line.

Suhas Nahas