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Yves Brun
Systems Biology/Microbiology Faculty Search
Department of Biology
Indiana University
Jordan Hall 142
1001 E 3rd St.
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Dear Dr. Brun:

It is my pleasure to write an enthusiastic and strong letter of recommendation for Dr. Yaroslava Yingling for a faculty position at Indiana University. Yara has a multi-disciplinary background that is reflected in her current research interests. Yara joined my group in 1997 through the Intercollegiate Graduate Program in Materials (IGPM) rather than Chemistry because her undergraduate training was in computer, physics and engineering related fields. Her background positioned her to undertake one of the most scientifically and computationally demanding projects in my group. Moreover, along the way she taught herself the essential organic and biological chemistry needed to develop a computational model of photochemistry. After leaving Penn State, she has taken a postdoc at the National Cancer Institute in computational studies of structure-function relationships of RNA.

Our group developed a mesoscopic molecular dynamics (MD) model for laser ablation and had successfully applied it to laser irradiation of organic solids in which the photon energy, typically in the UV, goes entirely into vibrational excitation of the molecules prior to Yara joining the group. Another possible mode of excitation is for the high-energy photons to induce a photochemical reaction, typically a bond scission event such as $C_6H_5Cl + h\nu \rightarrow C_6H_5\bullet + \bullet Cl$. As an aside, the physics of ablation in the corrective vision eye surgery, LASIK, is dominated by laser induced photochemistry. Following the initial photochemical event there are a number of subsequent reactions that can and do occur. Computationally, the challenge is to develop a methodology to examine the effects of these photochemical reactions on the ablation processes without completely getting bogged down in an overly massive theoretical and computational effort.

Yara has creatively tackled this complex modeling task. Her strategy was to delineate the possible chemical reactions following the initial bond scission event. The energies of the reactions were determined and properly incorporated into the simulation. In addition, probabilities of the various reactions were determined. I must point out that the prescription of how to incorporate such complex processes into a MD simulation without an atomistic representation of particles is not straightforward and had not been tackled before. The task of even determining and finding the relevant experimental data for making such decisions is tough and demands chemical intuition. Yara, independently, carefully developed the Course Grain

Chemical Reaction Model (CGCRM) for incorporating photochemical processes into the MD model. In addition she developed computational approaches to speed up her simulations. The simulations were and still are tour-de-force with each data point taking several weeks of computer time.

Yara has explained almost all of the experimental differences between pure thermal ablation of molecular solids and liquids and mixed photochemical-thermal ablation of similar materials. Moreover, her CGCRM calculations definitively show that the presence of exothermic abstraction and radical-radical recombination reactions drastically alters the energy balance in the system. Namely, with a pure thermal process, the energy available for ablation processes is given by the laser fluence and the depth profile by Beer's law. The exothermic reactions convert chemical potential energy into energy available for translational motion and heat, thus the effective energy available is greater than the laser fluence. The distribution of the energy deposition differs in depth and time from the pure thermal excitation processes. This concept, which had not been discussed previously, provides the essential basis for understanding the differences between photothermal and photochemical laser ablation. Delineating this physics would not have been possible without the detailed coarse grained model that Yara developed for laser ablation.

Yara's Ph.D. work has resulted in eight publications with her as first author including one article joint with experimentalists in Applied Physics Letters, an invited paper in the Journal of Photochemistry and Photobiology, and one article in Chemical Physics Letters. In addition, she contributed to three review papers including invited papers in Chemical Reviews and a special issue of the International Journal of Mass Spectrometry in honor of Franz Hillenkamp. Yara organized and wrote all of her papers. She gave her first talk on the work in 2000 at the national meeting of the American Society of Mass Spectrometry with over 100 people in attendance. In addition, she gave a talk at an international meeting on computer simulations in 2000 and a poster at a Gordon Research Conference in 2002. Both talks were excellent and very well received. Her command of English is excellent. In April 2003 she was chosen to receive the "best thesis" of the year award in the Materials Research Institute at Penn State.

Yara chose to remain in my group as a postdoc for an additional year because of issues involving her two children. On her own she chose to develop the CGCRM for modeling ablation of polymers. The model she had developed for her thesis carries over quite nicely to more complex and extended systems. As her parting gift to me, she wrote a NSF-ITR proposal that has been funded for modeling laser ablation of polymers. She also wrote the backbone of the code and has performed and published the initial simulations. I currently have a graduate student and postdoc working on her model.

Yara has a deep and sincere commitment to science. She multi-tasks very well. The IGPM requires numerous courses including many in engineering and materials science and has many hoops through which the students must jump. She also completed the required five courses for a graduate minor in High Performance Computing Applications. Throughout her time here, however, she stayed focus on her research.

Yara Yingling is an extremely creative and independent researcher. She developed the CGCRM on her own and developed the strategies for obtaining the information she needed as input. As computational issues arose, she figured out the best approach for solving the important issues. At all times she stayed focused on obtaining scientific results that can be compared to experimental data. Subsequent to her time here, she confidentially took a postdoctoral position at NCI to broaden her research experience to biological systems.

Yara Yingling is a scientist of the quality of some of my best graduate students and postdocs of the past - Don Brenner (NCSU), Leonid Zhigilei (U of VA), and Deepak Srivastava (NASA, Ames, CA). She has the creativity, drive and inherent abilities to contribute to a broad range of interesting and scientifically challenging problems. I wholeheartedly and enthusiastically recommend her for your faculty position at Indiana University.

Sincerely,

Barbara J. Garrison
Shapiro Professor of Chemistry

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