Abstract: Determining the orientation and conformation of an adsorbed biomolecule at an inorganic interface remains a grand challenge in studies of interest to materials science, medicine and biotechnology. Lack of a general approach, either computational or experimental, to study structure thermodynamics and kinetics of the bio/nano interface, advances in the field are often left to chance discovery vs detailed mechanistic understanding. Throughout this seminar I will present recent advances from our group in fundamental science and engineering of interfacial phenomena of complex peptides. The talk will present computational methods for determining the structure and thermodynamics of a bound peptide, experimental validation of the accuracy of the methods, and a series of examples of increasing complexity including titania binding peptides, proteins involved in the mineralization of bone and integration of implants, and synthetic peptides that are used to create hybrid bio/nano structures for hierarchical and multifunctional materials.

Education and training statement. Data science and associated methods like machine learning and AI continue to find new and exciting applications in fields like chemical and nanoengineering. In parallel, there are countless new job opportunities for domain scientists with knowledge of nanoscale systems and data science skills. At the end of my talk, I will discuss our data science training programs at the University of Washington and suggestions for students and postdocs who are interested in exploring career pathways in this new area.

Biosketch: Jim Pfaendtner is the Rogel Professor & Chair of Chemical Engineering at the University of Washington and Staff Scientist at Pacific Northwest National Laboratory. He holds a B.S. in Chemical Engineering (Georgia Tech, 2001) and a PhD in Chemical Engineering (Northwestern University, 2007). He also serves as Associate Vice Provost for Research Computing at the UW. Jim’s research focus is computational molecular science and his recent teaching interests are in the area of teaching data science skills to grad students in chemical and materials science and engineering. Jim is currently the director of an NSF graduate training program (NRT) at the intersection of data science and molecular science.