Introduction

This course introduces the concepts of computational chemistry, biochemistry, and materials science through a sequence of projects. The projects are linked by a common theme. This semester's theme is understanding chronic beryllium disease. This topic has links to chemistry, biochemistry, and materials science. First, we'll go through the syllabus and then I'll tell you a bit more about beryllium, chronic beryllium disease, and how we are going to learn about the techniques of computational science through a series of projects linked to this disease. See syllabus.

Beryllium

Beryllium is the fourth element in the periodic table. It contains four protons and four electrons. It has an atomic mass of about 9 atomic units. It's a lead gray metallic solid with some unique properties. As a result of its low density, high melting point, nuclear properties, and stability, beryllium is used in aerospace, ceramics, electronics, nuclear energy and defense, metal recycling industries, dentistry, and even sporting goods. It is also a key component in emeralds (beryl).

Beryllium is a very useful substance. However, industries processing beryllium, beryllium oxide, and beryllium/copper alloy have seen a significant number of workers become beryllium sensitized and develop chronic beryllium disease.

Chronic beryllium disease

Exposure to beryllium oxide by inhalation from beryllium, beryllium oxide, and beryllium/copper alloy processing plants has been linked to chronic beryllium disease (CBD). Once the beryllium oxide particulates are deposited on the lung membrane, macrophages engulf the particles. In the low pH (about 4.8) of the macrophage's lysosomal digestive fluid, beryllium oxide dissolves. Infected macrophages aggregate and form granulomas at the surface of the lungs. Scar tissue from the granulomar formation and inflamation from the immune response reduce the breathable lung tissue. This causes breathing difficulties and eventually death. Currently, there is no cure.

Working towards a cure requires collaboration from a variety of different disciplines – biology, chemistry, physics, materials science. Most of these disciplines are represented in the population of this class. I would like to use this these as a jumping off point to learn about scientific simulations and at the same time explore an unsolved problem. Let's introduce ourselves so we can get a sense of our different background. Introductions.

We'll start our exploration of this disease with a packet of key papers on the disease and on the materials involved. Read the articles. Next time, we'll discuss some more particulars of the disease, the most likely material involved, and the series of computational projects we'll use to clarify what occurs from the point of inhalation and beyond.