

Some possible investigations with the ion Coulomb crystal simulator

- 1) Properties of linear chain of ions.
 - A) For two up to ten ions, check that the ion separations are as predicted in “James Appl Phys 1998”.
 - B) For a selection of the number of ions in the chain, compare with the calculated minimum separations in “James Appl Phys 1998”.

- 2) Structural phase transitions.
 - A) For a selection of the number of ions, determine the critical ratio of the two trap frequencies for transitions between linear chains and zig-zag configurations, and compare with the results in “Dubin PRL 1993/Schiffer PRL 1993”
 - B) For a selection of the number of ions, determine the critical ratio of the two trap frequencies for transitions between 2D “pancake” structures and 3D configurations, and compare with the results in “Dubin PRL 1993/Schiffer PRL 1993”

- 3) Minimum energy states for spherical Coulomb crystals
 - A) Determine Magic numbers for the progressing shell structures, and compare with “Avilov_Hasse / Bonitz PhysRevE.71.046403”.
 - B) For cases where the two papers disagree on the minimum energy states, try to find out who is right!

- 4) Melting of Coulomb crystals.
 - A) Make a qualitative survey of how the melting point changes with the number of ions in spherical crystals. How does this match the results in “Schiffer PRL 2002”
 - B) Is there any dependency on aspect ratio of the crystals?

- 5) Make simulations of multi-species crystals
 - A) Can you produce a near-equidistantly string of $^{24}\text{MgH}^+$ ions inside a larger $^{40}\text{Ca}^+$ ion crystal
 - B) Can you reproduce the two-species crystal inside the glass bar?
 - C) How small a mass difference can you have and still get radial separation of two species?
 - D) Can you produce a three species crystal consisting of a string of one species, a cylindrical shell of another inside of an outer third species?

Note: The relevant articles can be found in the folder “Some background literature for MD simulations”. In each article the important parts for the exercises above are marked by yellow.