Computer Simulations of Glasses

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Abstract:

Some people consider computer simulations to be a magic wand that is able to solve all the problems in glass science. Others see is as a fancy but basically useless tool with no predictive power. In this talk I will briefly discuss the technique of computer simulations and give some examples which show that simulations can indeed be useful to gain a better understanding of glasses. However, there are pitfalls in this technique, some of them can be avoided and some not, and I will present some of these problems in order to allow each member of the audience to judge by him/herself whether or not a given simulation should be considered as faulty or useful.

Questions to be answered:

1.) What will be a topic stating an exceptional success to be published in a well known high ranking Research Journal in 2025 concerning your presented R&D field of work? Please think in headlines.

Ab initio simulation of 10 million particles

2.) Please name up to 10 future key challenges (till 2025) regarding your presented field of expertise and indicate please the specific year when you expect the topic to become a real bottleneck for the future developments.

Note
- most of the years I state in which the challenges will become a bottleneck are "2009=now", i.e. there is currently not enough progress to allow to answer the relevant questions.

- I have formulated the challenges in a way that it is clear what has to be done in order to get a breakthrough.

1) how to make simulations in equilibrium at temperatures around T_g (now)

2) corrosion of glass by water (now)

3) long time behavior of nuclear glasses (now)

4) understanding the mechanism responsible for the slowing down of glass-forming systems and thus the glass-transition (now)

5) crack propagation in glasses (now)

6) simulating nanoparticles in an amorphous matrix (now)

7) how to connect different length and time scales in multi-scale simulations (2015)

8) how to obtain transferable classical interaction potentials for "arbitrary" compositions (2013)

3.) Concerning the topics, what would be

a) the key breakthrough and when is it likely to occur

b) what must happen concerning the research field if this topic will never be successful

a) 1) and 8)
b) These problems **will** be solved