

AIMD study of the cooling rate effect on the physical properties of amorphous GeS₂: evidences of the broken chemical order in glasses

and

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If the temperature of a liquid is decreased so much that the relaxation time of the system becomes longer than the time scale of the computer simulation or of the experiment, the system undergoes a kinetic arrest and, provided that it does not crystallize, will undergo a glass transition and remain trapped in a disordered configuration. However, it has been demonstrated in both experiment [1,2] and computer simulations [3,4] that the properties of the resulting glass, like the density or the glass transition temperature, will depend on its thermal history and in particular on the rate at which the sample is cooled down.

Using ab-initio molecular dynamics simulations we study the cooling rate effects on the physical properties of amorphous germanium disulfide GeS₂. The effects on the structural and electronic properties are analyzed.

[1] Brüning R and Samwer K 1992 Phys. Rev. B 46 11318–22

[2] Brüning R and Sutton M 1994 Phys. Rev. B 49 3124–30

[3] Miyagawa H and Hiwatari Y 1989 Phys. Rev. A 40 6007–13

[4] Vollmayr K, Kob W and Binder K 1996 Phys. Rev. B 54 15808–27

Host: Juan Peralta

Cookies and coffee @ 3:30pm in Dow 201.