

Abstract Submitted
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**Dynamics across the liquid-liquid transition in Si and Ga:
The fragile-to-strong transition**¹ SAMUEL CAJAHUARINGA, MAURICE DE
KONING, ALEX ANTONELLI, UNICAMP-Univ de Campinas — The existence of
liquid-liquid phase transitions (LLPT) has been proposed to explain the anomalies
in thermodynamic properties of substances such as, water, Si, Ga, etc. Recently,
there has been an increasing interest in the liquid dynamics near LLPTs. It has
been also suggested the occurrence of a fragile-to-strong transition (FTST) in the
dynamics of water and Si accompanying the LLPT. Using computer simulations
we study the dynamics of two atomic liquids that display a LLPT: Si and Ga. In
particular, our goal is to investigate to what extent the presence of a dip in the
self-intermediate scattering function (SISF) is caused by an excess of vibrational
states at low frequencies, which may be associated with a FTST across the LLPT,
as suggested recently. Our results do not provide support to these suggestions. In
the specific case of Ga, we observe the appearance of an excess of vibrational states
at low frequencies, even though the development of a dip in the SISF across the
LLPT is not observed. Moreover, our study of the shear viscosities traversing the
LLPTs indicates that, despite the appearance of a dip in the SISF for the case of Si
and its absence in Ga, both substances exhibit a fragile character above and below
the LLPT temperatures.

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Alex Antonelli
UNICAMP-Univ de Campinas

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