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Preface

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In a recent issue of Science (Science, Vol. 267, 1616 (1995)), Nobel laureate P. W. Anderson commented, "The deepest and most interesting unsolved problem in solid state theory is probably the theory of the nature of glass and the glass transition. This could be the next breakthrough in the coming decade." If such a breakthrough is indeed in the offing, is it possible to predict today the form that this advance will take? In particular, is it possible to anticipate if and how computer simulations might play a role in this breakthrough? What are the necessary requirements for a minimal model of the glass transition? And from the standpoint of applications, how far are we from a *technologically useful* theory of glass formation - one that leads to significant improvements in the wide range of technologies that depend on understanding the diverse aspects of the glassy state of matter?

These were the questions addressed by a handful of leading researchers at a recent workshop entitled "Glasses and the Glass Transition: Challenges in Materials Theory and Simulation." The workshop was held this past February at the Kent Manor Inn in Stevensville, MD under the auspices of the NIST Center for Theoretical and Computational Materials Science [1]. The goal of the workshop was to establish the current status of our understanding of this technologically important and intellectually fascinating field through three days of presentations and roundtable discussions.

The workshop brought together a diverse set of people that included experimentalists, theoreticians, and computer simulationists. While the starting point of the workshop was the phenomenology of glasses, the diverse mix of participants led to a rapid realization that the perception (or definition) of glassy behavior is often in the eye of the beholder. We found it easy to identify common characteristics of the glassy state, yet difficult to construct a precise definition of glasses or the glass transition. The exchange of perceptions led to an improved understanding of the gaps in the current state of knowledge. These gaps are addressed by a number of participants in these proceedings.

Of the many issues discussed at the meeting, a key point raised was the need for a minimal theoretical model of a glass that would play the same role in the study of glasses that, e.g., the Ising model plays in the study of critical phenomena in magnets and fluids. Such a generic glass model is needed to elucidate both the nature and universality of the glass transition, as well as to provide qualitative understanding of experimental results. Several candidate models were extensively discussed, including specialized interaction potentials for liquids, percolation models, and spin models. In all cases, it was demonstrated that computer simulation studies of these models is playing a leading role in their development.

[1] A list of relevant papers submitted by the participants prior to the workshop can be found on the CTCMS Materials Theory Information Web Server (http://www.ctcms.nist.gov).

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Contained in this proceedings are the reflections and viewpoints of the participants of the workshop on key experimental developments, theoretical advances, and especially the role of computer simulations, in the quest for a universally accepted, comprehensive, and technologically useful theory of the glass transition. Authors were asked to be informal and provocative, and this is reflected in the various manuscript styles and opinions contained in these pages. We are grateful to the attendees for their enthusiastic participation — it is hoped that these proceedings will stimulate further debate and research effort in this exciting and challenging field.