system through which a shockwave (such as that generated by detonation) propagates, they only apply QMD to a smaller region around a shockfront, which changes as the wave moves through the system. This provides several more orders of magnitude improvement in computational efficiency.

QMD not only provides information about the dynamical evolution of a system's atomic structure but also its electronic structure. This is very important for investigating the occurrence of a transition from an insulating to a conducting state (metallization) during the detonation. Gilman[5] suggested that the shock-wave front in detonations may cause local metallization in covalently bound explosive systems such as nitromethane. As a first indication of such behaviour, Reed *et al.*[2] observe the occurrence of 'bandgap filling' in the density-of-states time evolution. This is not, however, sufficient for the evidence of metallization. The definitive criterion for metallization is given by the estimation of Mott's electronic state overlap parameter[6]. This criterion is only fulfilled during a narrow time window (30 ps) and the limit of the doped semiconductor metallization is not reached (see Fig. 1). Reed *et al.* interpret this behaviour as resulting from the formation of a semimetallic state, taking place within a transient layer behind the detonation shock front of the explosive nitromethane.

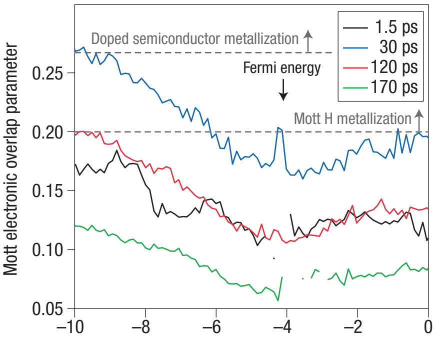


**Figure 1** Evidence for the occurrence of an insulator–metal transition during quantum molecular dynamics simulation of the detonation of nitromethane[2]. Part of the power of the use of quantum molecular dynamics simulations is that they provide both structural and electronic information. This enables Reed *et al.*[2] to estimate the so-called Mott overlap parameter[6] — which quantifies whether a system is a metal, a semiconductor or an insulator — as a function of energy for the electronic structure of an ensemble of nitromethane molecules at different times during detonation. It has been suggested that a covalent explosive such as nitromethane may undergo a transition from insulating to metallic behaviour during detonation, though Reed *et al.* only observe a transition to a state equivalent to a doped semiconductor for a brief moments of around 30 ps during their simulation.

It is also notable that the results of the simulations are consistent with recent experimental observations[7]. But despite the fact that nitromethane (and its detonation properties in particular) having been thoroughly investigated by others makes it a good choice for testing the authors' simulation approach, it might not necessarily be the best candidate for the observation of a Mott (metal–insulator) transition in the shock-wave front of a detonation. In my view, explosives with a negative oxygen balance, such as TNT (trinitrotoluene) or Hexogen (cyclotrimethyltrinitramine) that are in more common usage as practical explosives are much better candidates for observing such effects. In demonstrating that it is now possible to use QMD to simulate a detonation event, the present work will hopefully encourage others to explore the physics of explosive chemistry.

### References

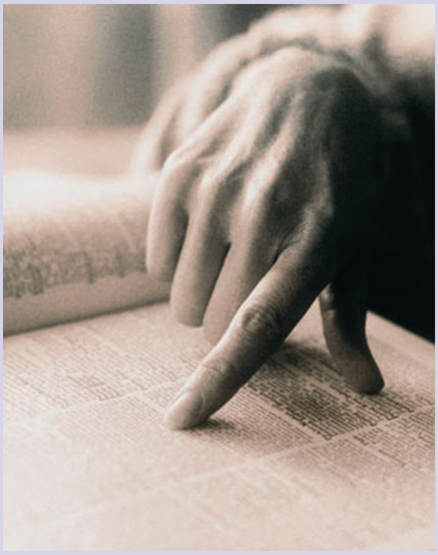
1. de Carli, P. S. & Jamieson, J. C. *Science* **133,** 1821–1822 (1961).
2. Reed, E. J., Manaa, M. R., Fried, L. E., Glasesemann, K. R. & Joannopoulos, J. D. *Nature Phys.* **4,** 72–76 (2008).
3. Engelke, R. *et al. J. Phys. Chem. A* **110,** 7744–7748 (2006).
4. Reed, E. J. *et al. Phys. Rev. Lett.* **90,** 235503 (2003).
5. Gilman, J. J. *Science* **274,** 65 (1996).
6. Mott, N. F. *Proc. R. Soc. London* **A382,** 1 (1982).
7. Gilev, S. D. & Trubachev, A. M. *Tech. Phys.* **46,** 1185–1189 (2001).

## STRING THEORY

# Stringlish lessons

It is much touted that string theory — although offering an excess of solutions, and thereby possible universes — has yet to make a testable prediction. The energy scales involved are so huge that no useful laboratory experiment can be envisaged. Even the fact that, at low energies, any such theory would have to reproduce the well-tested standard model of particle physics proves little help in trying to identify a viable string-theory solution in the landscape of myriad possibilities.

But any such solution would also have to reproduce the observed cosmology of our Universe: now that we have some knowledge of the early history of the Universe, particularly through observations of the cosmic background radiation, perhaps here there are better clues to be found. Writing in *Physical Review D*, Mark P. Hertzberg and colleagues consider the case of inflation and whether string theory can indeed account for this period of exponential expansion, believed to have occurred in the very earliest stages of the Universe's development (*Phys. Rev. D* **76,** 103521; 2007).


GETTY

First, Hertzberg *et al.* acknowledge that there is a significant language barrier to communication between string theorists on one side and astrophysicists on the other. To aid astrophysicist readers, they include a short dictionary of 'stringlish', translating string-theory jargon such as 'orientifold *p* plane' and 'Kähler potential' into phrases that astrophysicists might be a little more comfortable with.

The authors investigate three string-theory models as examples, checking for the necessary conditions to achieve 'slow-roll' inflation. Although a full computation in each case was unfeasible, so they do not claim the results as hard proof, Hertzberg *et al.* nevertheless find that in none of the models does inflation occur.

All is not lost, however. This study indicates that, as the authors put it, "slow-roll inflation may be a rare and delicate phenomenon in the landscape", but it also signals that there may be better places to look — in other regions of the landscape where the obstacles to inflation found so far might not exist. String theorists and astrophysicists may proceed together, stringlish dictionary in hand.

**Alison Wright**