## Phase behaviour of colloid + polymer mixtures

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**Abstract**

A new treatment of the phase behaviour of a colloid + non-adsorbing polymer mixture is described. The calculated phase diagrams show marked polymer partitioning between coexisting phases, an effect not considered in the usual effective-potential approaches to this problem. The authors also predict that under certain conditions an area of three-phase coexistence should appear in the phase diagram.

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## Superconductivity, spin gaps and Luttinger liquids in a class of cuprates

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**Abstract**

A homologous series of cuprates can be formed by introducing a parallel array of planar defects into the infinite-layer cuprate, $SrCuO_2$. In each $CuO_2$ plane line defects consisting of CuO double chains result. Analysis of the electronic properties of such planes is demonstrated. When lightly doped with holes the spin gap will remain and singlet superconductivity should occur on a separate but high temperature scale. This prediction may shed new light on the origin of the separate energy scales for the spin gap and superconductivity in other lightly doped cuprates.

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## Interatomic potentials from first-principles calculations: the force-matching method

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**Abstract**

We present a new scheme to extract numerically "optimal" interatomic potentials from large amounts of data produced by first-principles calculations. The method is based on fitting the potential to *ab initio* atomic forces of many atomic configurations, including surfaces, clusters, liquids and crystals at finite temperature. The extensive data set overcomes the difficulties encountered by traditional fitting approaches when using rich and complex analytic forms, allowing to construct potentials with a degree of accuracy comparable to that obtained by *ab initio* methods. A glue potential for aluminium obtained with this method is presented and discussed.

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## Size-dependent depression of the glass transition temperature in polymer films

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**Abstract**

The glass transition temperature of thin polystyrene films has been measured as a function of film thickness. It is found that the glass transition decreases in temperature as the thickness of the film is reduced. The effect is not strongly molecular-weight dependent, ruling out chain confinement as the major cause; instead we suggest that at the surface of the glassy film a liquidlike layer exists whose size diverges as the glass transition temperature is approached from below.

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## Stability and band gap constancy of boron nitride nanotubes

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**Abstract**

Extensive LDA and quasi-particle calculations have been performed on boron nitride (BN) single-wall and multi-wall nanotubes. Strain energies are found to be smaller for BN nanotubes than for carbon nanotubes of the same radius, owing to a buckling effect which stabilizes the BN tubular structure. For tubes larger than 9.5 Å in diameter, the lowest conduction band is predicted to be free-electron-like with electronic charge density localized inside the tube. For these tubes, this band is at constant energy above the top of the valence band. Consequently, contrarily to carbon nanotubes, single- and multi-wall BN nanotubes are constant-band-gap materials, independent of their radius and helicity. In addition, we expect them to exhibit remarkable properties under *n*-type doping.

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