Centro de Investigaciones Ópticas
Más de 30 Años de Investigación en Ciencia y Tecnología

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Ab initio studies of ultrafast structural changes in femtosecond laser excited materials

Tobias Zier
Diploma in physics at the University of Kassel.
Kassel, Germany

***Abstract*:** Femtosecond laser pulses can be used to practically instantaneously manipulate bonds in solids through the creation of a hot electron plasma. At sufficiently high fluences, some phonon modes may even become unstable, causing acceleration of the atoms, followed by a disordering within several 100's of femtoseconds. This ultrafast solid-to-liquid phase transition is called nonthermal melting and has been observed in silicon, germanium, gallium arsenide, indium antimonide, and bismuth. It is, however, not known which physical process leads up to nonthermal melting at fluences below the melting threshold and which pathways are followed by the atoms after a high intensity excitation. With our ab initio density functional theory code CHIVES we were able to simulate these situations, which are far from thermodynamic conditions and address this open questions. Further I will show some selected topics of my PhD work

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Camino Parque Centenario y 506, M. B. Gonnet C.C. 3 (1897) • La Plata - Buenos Aires – Argentina
TE: +54 221 484-0280 / 2957; +54 221 471-5249 • Fax: +54 221 471-2771 • e-mail: info@ciop.unlp.edu.ar