

Oxygen diffusion through disordered SiO₂

Angelo Bongiorno and Alfredo Pasquarello

*Institut de Théorie des Phénomènes Physiques (ITP), Ecole Polytechnique Fédérale de
Lausanne (EPFL), CH-1015 Lausanne, Switzerland*

*Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA),
CH-1015 Lausanne, Switzerland*

An atomic-scale description is provided for the long-range oxygen migration through disordered SiO₂. First-principles calculations, classical molecular dynamics, and Monte-Carlo simulations are used in sequence to span the relevant length and time scales. The O₂ molecule is firmly identified as the transported oxygen species and is found to percolate through interstices without exchanging oxygen atoms with the network. The interstitial network for O₂ diffusion is statistically described in terms of its potential energy landscape and connectivity. The associated activation energy is found in agreement with experimental values.