

Abstract Submitted
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PIMC simulation of Ps in a dielectric solid ZACHARY WOLFSON,
Swarthmore College, AMY BUG, Swarthmore College — Positronium (Ps) is commonly used to probe the pore space in insulating materials like polymers and low-k dielectrics. Such studies require an accurate model relating the lifetime to the size of the pore. The standard Tao-Eldrup approach models Ps as one quantum particle in the ground state of a spherical box. We go beyond Tao-Eldrup by modeling Ps exactly as two quantum particles at arbitrary temperature, using Path Integral Monte Carlo (PIMC) to simulate the electron and positron each as a classical polymer. As a further correction, we also include the dielectric response of the surrounding material. The total annihilation rate, which is the inverse of the lifetime, may be calculated from the pickoff and self annihilation rates via

$$\Gamma = \Gamma_{p.o.} + \kappa\Gamma_{self}$$

We find that the material's polarization causes the Ps to be more attracted to the wall, decreasing its pickoff lifetime. The internal contact density, κ , decreases with increasing dielectric constant. The combination of using the two particle model as well as polarizable walls yields a lifetime close to the Tao-Eldrup result.

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