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Machine learning modeling for infrared spectra of titanium carbide nanoparticles

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Titanium carbide (TiC) nanoparticles are believed to be among the first solid compounds to condense in the outflows of carbon rich evolved stars, acting as nucleation seeds for cosmic carbonaceous dust. These tiny but crucial grains may influence the chemical evolution of galaxies by catalyzing the formation of complex organic molecules in space. A key challenge is identifying such grains observationally and that hinges on the accurate prediction of their infrared (IR) spectral signatures. While density functional theory (DFT) has been a powerful tool for simulating the vibrational and IR spectra of nanostructures, it remains computationally demanding, especially for large or dynamic systems. Machine learning (ML) emerges as a compelling alternative, promising accurate predictions at a fraction of the cost. Yet, its adoption in astrochemistry remains limited, in part due to concerns about the reliability of ML models in reproducing detailed physical behavior. In this contribution, we present a machine-learned interatomic potential trained on DFT molecular dynamics trajectories of TiC nanoparticles, using the MACE architecture. The ML-generated IR spectra show excellent agreement with DFT benchmarks and are transferable to larger nanoparticle sizes. This opens up exciting possibilities for simulating astrophysical dust populations with realistic dynamics and scale a necessary step toward bridging the gap between theoretical modeling and observational astronomy.