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Diffusion of Interacting Particles in Discrete Geometries KWIN-TEN NELISSEN, Universiteit Antwerpen, 2020 Antwerp, Belgium, T. BECKER, BART CLEUREN, Hasselt University, 3590 Diepenbeek, Belgium, B. PARTOENS, Universiteit Antwerpen, 2020 Antwerp, Belgium, C. VAN DEN BROECK, Hasselt University, 3590 Diepenbeek, Belgium, CMT COLLABORATION, THEORETI-CAL PHYSICS COLLABORATION — We evaluate the self-diffusion and transport diffusion of interacting particles in a discrete geometry consisting of a linear chain of cavities, with interactions within a cavity described by a free-energy function. Exact analytical expressions are obtained in the absence of correlations, showing that the self-diffusion can exceed the transport diffusion if the free-energy function is concave. The effect of correlations is elucidated by comparison with numerical results. Quantitative agreement is obtained with recent experimental data for diffusion in a nanoporous zeolitic imidazolate framework material, ZIF-8.

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