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# Understanding the effect of defects on $^{3}$He diffusion in quartz with paired simulations and experiments

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We present preliminary results from a study to systematically investigate the role of defects in modulating $^{3}$He diffusion in quartz. At Earth's surface, $^{3}$He is produced in quartz by interactions with cosmic ray particles and diffusively lost from quartz at surface temperatures. This concurrent production and diffusion of $^{3}$He can be used to constrain past surface temperatures if the diffusion kinetics of $^{3}$He are known. Laboratory diffusion experiments on different quartz samples exhibit inter-sample variability in $^{3}$He diffusion kinetics, with some samples exhibiting complex $^{3}$He diffusion behavior. Previous density functional theory (DFT) calculations demonstrate that extended defects that disrupt the *c*-axis channels in quartz, such as nanopores, can play an important role in modulating the diffusion of $^{3}$He, which may explain the variability of $^{3}$He diffusion kinetics observed in laboratory experiments. However, there has been no direct link between defects modeled in DFT calculations and defects known to be present in quartz samples studied in laboratory diffusion experiments. Here, we pair laboratory $^{3}$He diffusion experiments on well-characterized synthetic and gem-quality natural quartz samples with DFT calculations, wherein the specific defects known to be present in samples are simulated. We will present (1) a suite of spectroscopic data that we use to characterize the type and abundance of defects present in our quartz samples, (2) predictions for the effects of these defects on $^{3}$He diffusion kinetics from DFT calculations, and (3) preliminary results from laboratory diffusion experiments on these samples. Ultimately, we aim to synthesize the DFT calculations with our laboratory experiments on well-characterized samples in order to provide a mechanistic explanation for variable and sometimes complex $^{3}$He diffusion behavior in quartz.