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Methods to Discover New Photocathode Materials using Machine Learning and Data-Driven Screening

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The photocathodes used as electron sources in high-performance electron accelerators today are largely one of only a handful of materials. While there has been an increased understanding of the properties of the electron beams produced by these cathodes, there has been little change in the overall selection of materials used at accelerator facilities. In fact, nearly all of the photocathodes in use today originated in the photomultiplier tube or night vision goggle industries, where efforts were aimed at discovering new materials by employing trial-and-error based iterative experimental approaches.

Our work in the field of photocathode discovery was initially directed towards improving the brightness of electron beams used in FELs and was the first data-driven approach to screening for high brightness photocathode materials. Through screening over 74,000 semiconducting materials, a list of novel candidate materials was generated. Our current work is focused on two other areas of interest for photocathodes: very high average current photocathodes and spin-polarized electrons. We will apply active learning techniques to reduce the amount of computationally expensive calculations that need to be performed in order to discover more new materials for photocathodes.

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Footnotes

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