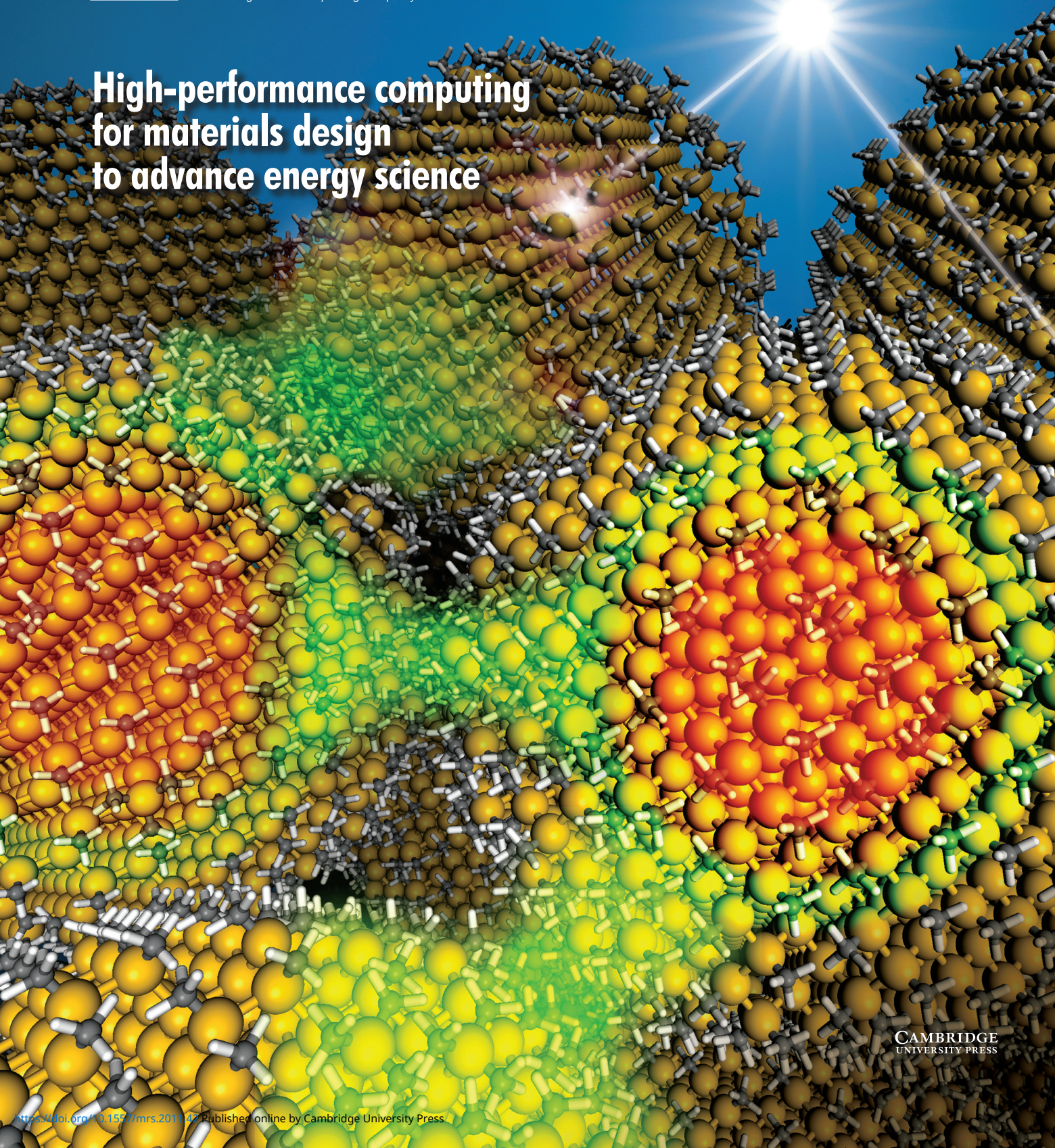


# MRS Bulletin



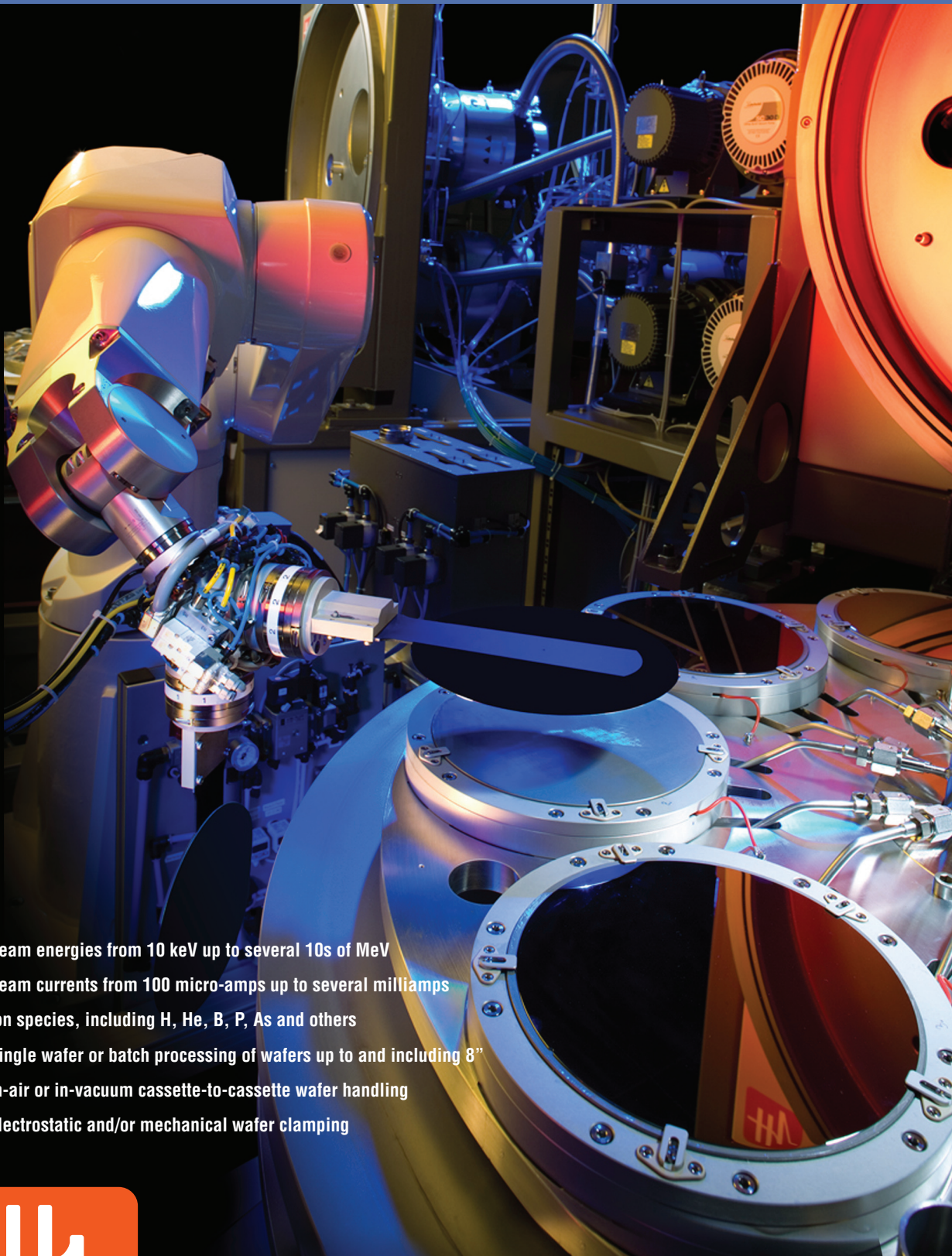
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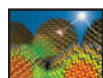


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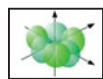
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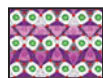
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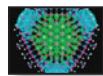
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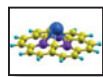
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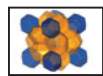
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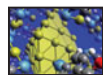
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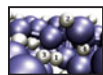
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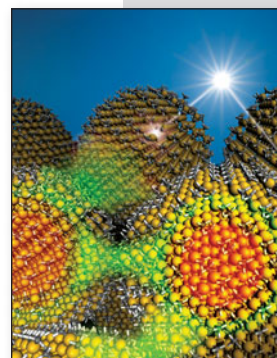
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## ON THE COVER



**High-performance computing for materials design to advance energy science.** This issue of *MRS Bulletin* explores the many ways in which high-performance computing is being used to design materials that improve the collection, conversion, and storage of energy. Such computational design projects typically scrutinize architectures and processes at the atomic level. For instance, the cover image illustrates the collection of solar energy by silicon atoms (small tan spheres) assembled into quantum dots (large spheres) that are then functionalized with ligands to shield them from oxidation and/or change their electronic properties. The dots shown are comprised of thousands

of silicon atoms and have diameters on the order of four nanometers. A given absorbed photon from the sun generates an exciton, a coupled electron-hole-pair depicted as diffuse, adjacent green and orange regions. This quasi-particle is initially confined to a single quantum dot but can subsequently tunnel to neighboring dots until it reaches a collection center. There the electron and hole are separated, resulting in an electrical current. The graphic was created by Mark Lusk, Department of Physics, Colorado School of Mines. See the technical theme that begins on p. 169.

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