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Positronium physisorption at quartz surfaces[1] ROLANDO SANIZ, ARTHUR FREEMAN, Northwestern University, BERNARDO BARBIELLINI, Northeastern University, PHIL PLATZMAN, Bell Laboratories — The possibility of having positronium (Ps) physisorbed at a material surface is of great fundamental interest, since it can lead to new insight regarding quantum sticking and is a necessary first step to try to obtain a Ps_2 molecule on a material host. Experimental evidence for physisorbed Ps at the surface of quartz was reported some years ago,[2] but firm theoretical support for such a conclusion was lacking. With the FLAPW method[3] we calculated the electronic structure and dielectric function of α-quartz and obtained the interaction potential with a Ps atom on its surface. We show that there is indeed a bound state with an energy of ~ 0.19 eV, which is reasonably close to the experimental estimates of 0.14 - 0.17 eV. A brief energy analysis in terms of the Langmuir-Hinshelwood mechanism further shows that the formation of a Ps_2 molecule at quartz surface would be possible.

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[2]Sferlazzo, Berko, Canter, Phys. Rev. B **3**, 6067 (1985).
[3]Wimmer, Krakauer, Weinert, Freeman, Phys. Rev. B **24**, 864 (1981).

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